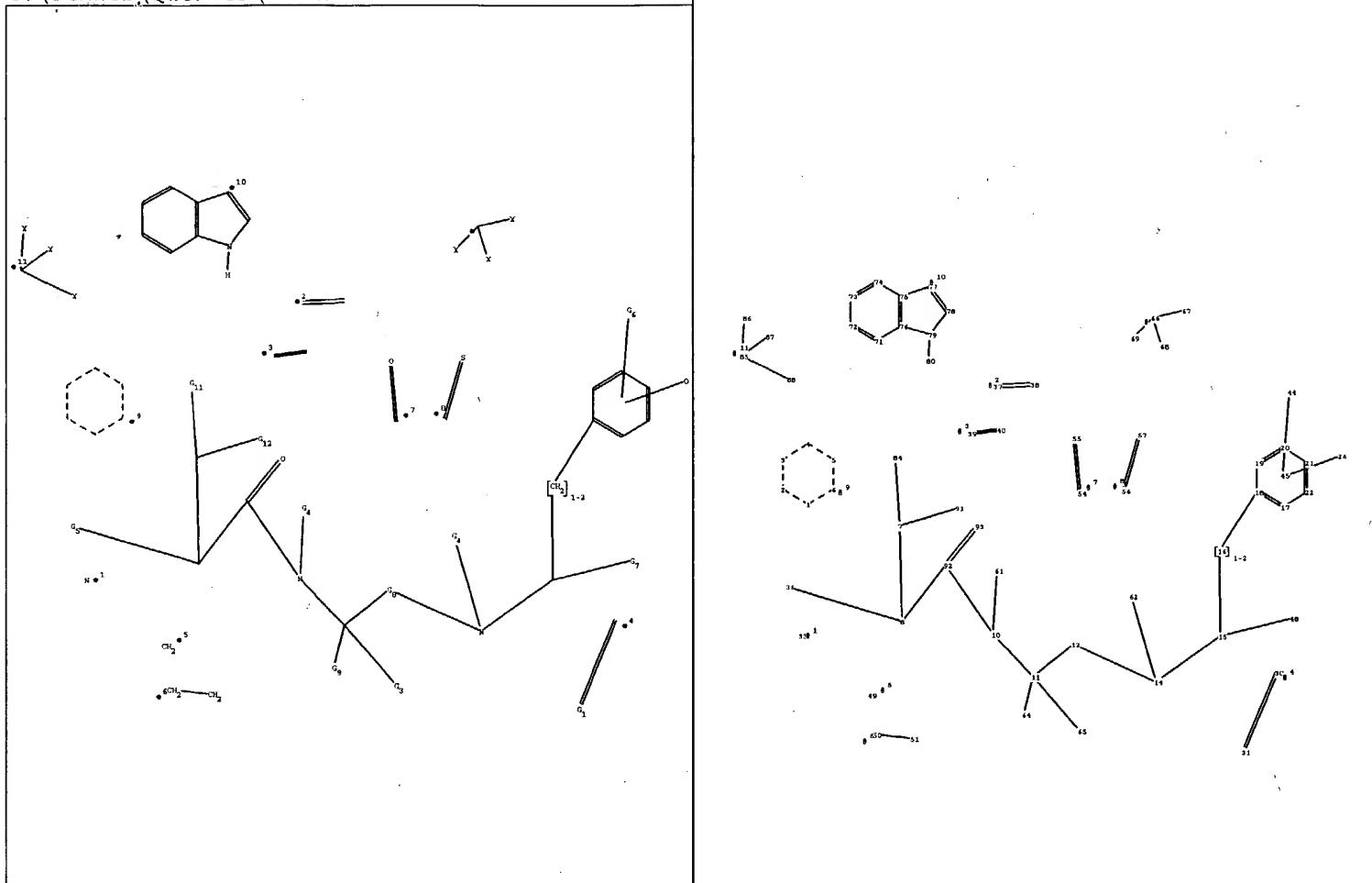


09-890217

C:\stnweb\Queries\1.str



chain nodes :

7 8 10 11 12 14 15 16 26 30 31 33 36 37 38 39 40 44 48 49 50 51 54  
55 56 57 61 62 64 65 66 67 68 69 80 84 85 86 87 88 91 92 93

ring nodes :

1 2 3 4 5 6 17 18 19 20 21 22 71 72 73 74 75 76 77 78 79

chain bonds :

7-8 7-84 7-91 8-36 8-92 10-61 10-11 10-92 11-12 11-64 11-65 12-14 14-15  
14-62 15-16 15-48 16-18 30-31 37-38 39-40 50-51 54-55 56-57 66-67 66-68 66-69  
79-80 85-87 85-88 85-86 92-93

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 17-18 17-22 18-19 19-20 20-21 21-22 71-72 71-76  
72-73 73-74 74-75 75-76 75-77 76-79 77-78 78-79

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-84 7-91 8-36 10-61 10-11 11-12 11-64 11-65 12-14  
14-15 14-62 15-48 30-31 54-55 56-57 76-79 78-79 92-93

exact bonds :

7-8 8-92 10-92 15-16 16-18 37-38 39-40 50-51 66-67 66-68 66-69 75-77 77-78  
79-80 85-87 85-88 85-86

normalized bonds :

17-18 17-22 18-19 19-20 20-21 21-22 71-72 71-76 72-73 73-74 74-75 75-76

isolated ring systems :

containing 1 : 17 : 71 :

G1:O,S

G2:CH3,Et

G3:H,Ak

G4:CH3,Et,H

G5:Ak,H,OH, [\*1]

G6:Ak,Cb, [\*2], [\*3]

G7: COOH, Ak, H, [\*4]

G8: [\*5], [\*6], [\*7], [\*8]

G9 : Ak , Ph

G11: [\*9], [\*10]

G12:H,OH,NH2,CN,[\*11]

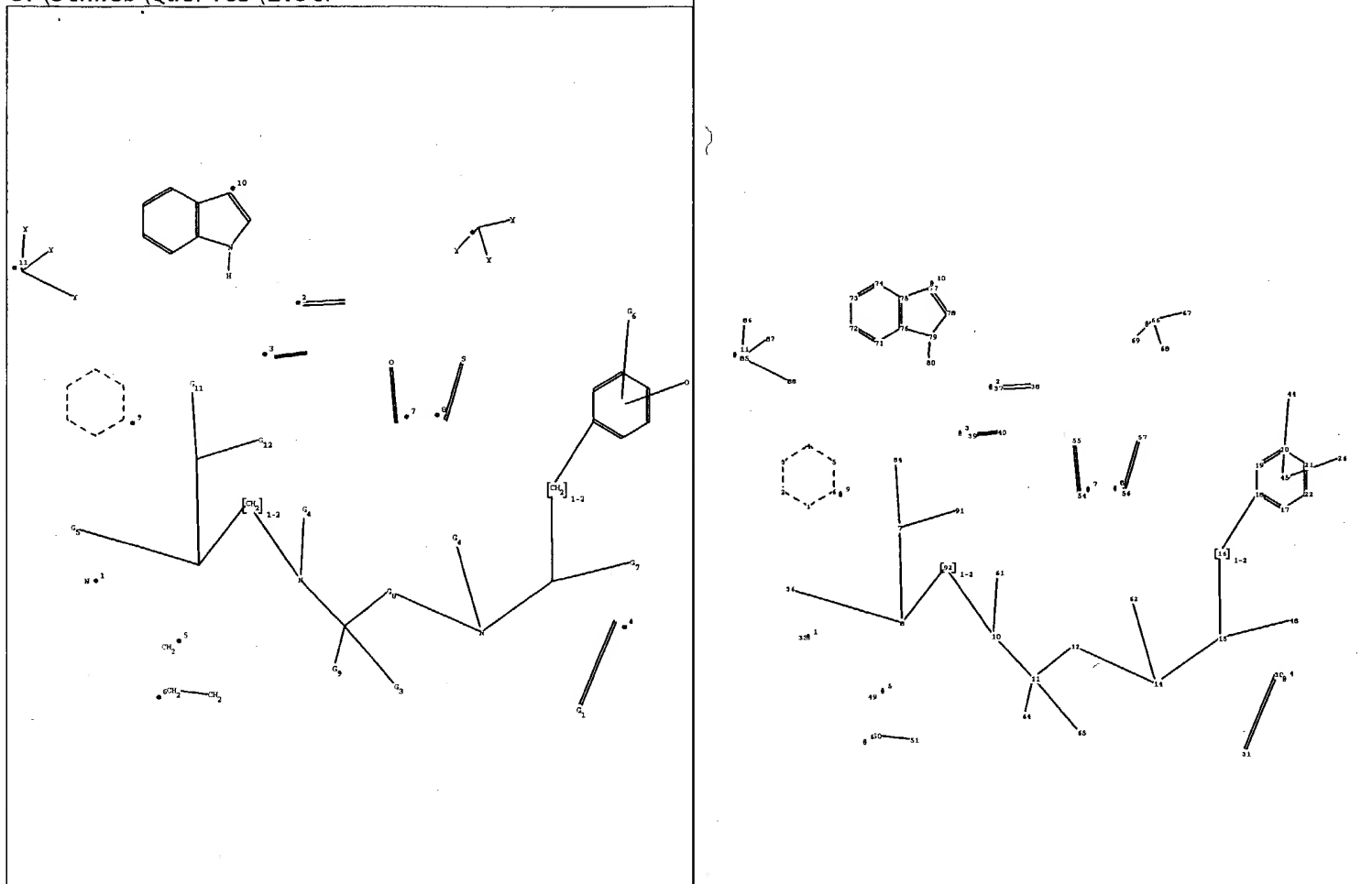
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1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 10:CLASS 11:CLASS
12:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 26:CLASS 27:CLASS 30:CLASS 31:CLASS 33:CLASS 36:CLASS 37:CLASS 38:CLASS
39:CLASS 40:CLASS 44:CLASS 45:CLASS 48:CLASS 49:CLASS 50:CLASS 51:CLASS 54:CLASS
55:CLASS 56:CLASS 57:CLASS 61:CLASS 62:CLASS 64:CLASS 65:CLASS 66:CLASS 67:CLASS
68:CLASS 69:CLASS 71:CLASS 72:CLASS 73:Atom 74:Atom 75:Atom 76:Atom 77:CLASS
78:CLASS 79:CLASS 80:CLASS 84:CLASS 85:CLASS 86:CLASS 87:CLASS 88:CLASS 91:CLASS
92:CLASS 93:CLASS

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C:\stnweb\Queries\1.str



chain nodes :

7 8 10 11 12 14 15 16 26 30 31 33 36 37 38 39 40 44 48 49 50 51 54  
55 56 57 61 62 64 65 66 67 68 69 80 84 85 86 87 88 91 92

ring nodes :

1 2 3 4 5 6 17 18 19 20 21 22 71 72 73 74 75 76 77 78 79

chain bonds :

7-8 7-84 7-91 8-36 8-92 10-61 10-11 10-92 11-12 11-64 11-65 12-14 14-15  
14-62 15-16 15-48 16-18 30-31 37-38 39-40 50-51 54-55 56-57 66-67 66-68 66-69  
79-80 85-87 85-88 85-86

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 17-18 17-22 18-19 19-20 20-21 21-22 71-72 71-76  
72-73 73-74 74-75 75-76 75-77 76-79 77-78 78-79

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-84 7-91 8-36 10-61 10-11 11-12 11-64 11-65 12-14  
14-15 14-62 15-48 30-31 54-55 56-57 76-79 78-79

exact bonds :

7-8 8-92 10-92 15-16 16-18 37-38 39-40 50-51 66-67 66-68 66-69 75-77 77-78  
79-80 85-87 85-88 85-86

normalized bonds :

17-18 17-22 18-19 19-20 20-21 21-22 71-72 71-76 72-73 73-74 74-75 75-76

isolated ring systems :

containing 1 : 17 : 71 :

G1:O,S

G2:CH3,Et

G3:H,Ak

G4:CH3,Et,H

G5:Ak,H,OH,[\*1]

G6:Ak,Cb,[\*2],[\*3]

G12:H,OH,NH2,CN,[\*11]

Match level :

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1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 10:CLASS 11:CLASS
12:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
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92:CLASS

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=&gt; \$ 195

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 SAMPLE SCREEN SEARCH COMPLETED - 456 TO ITERATE

100.0% PROCESSED 456 ITERATIONS 0 ANSWERS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 7839 TO 10401  
 PROJECTED ANSWERS: 0 TO 0

L96 0 SEA SSS SAM L95

=&gt; \$ 195 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS  
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:Y  
 FULL SEARCH INITIATED 22:40:54 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 9898 TO ITERATE

100.0% PROCESSED 9898 ITERATIONS 5 ANSWERS  
 SEARCH TIME: 00.00.01

L97 5 SEA SSS FUL L95

=&gt; file hcaplus

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	ENTRY	SESSION
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	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-7.00

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FILE COVERS 1907 - 2 Sep 2004 VOL 141 ISS 10  
 FILE LAST UPDATED: 1 Sep 2004 (20040901/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L98 1 L97

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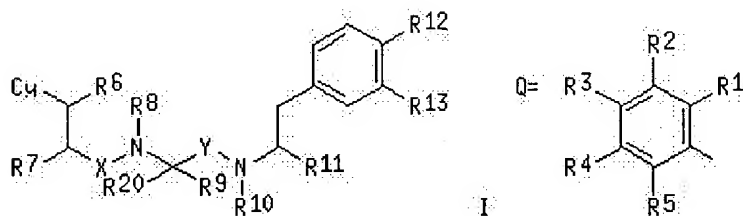
L98 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Chemical References
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ACCESSION NUMBER: 2000:535162 HCAPLUS  
 DOCUMENT NUMBER: 133:150920  
 TITLE: Preparation of peptides or analogs containing substituted phenethylamine moiety as motilin receptor antagonists  
 INVENTOR(S): Matsuoaka, Hiroharu; Sato, Tsutomu; Takahashi, Tadakatsu; Kim, Dong Ick; Jung, Kyung Yun; Park, Chan Hee  
 PATENT ASSIGNEE(S): Chugai Seiyaku Kabushiki Kaisha, Japan  
 SOURCE: PCT Int. Appl., 403 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

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<u>WO 2000044770</u>	A1	20000803	<u>WO 2000-JP444</u>	20000128
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<u>CA 2359030</u>	AA	20000803	<u>CA 2000-2359030</u>	20000128
<u>EP 1149843</u>	A1	20011031	<u>EP 2000-901956</u>	20000128
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
<u>NO 2001003684</u>	A	20010928	<u>NO 2001-3684</u>	20010726
PRIORITY APPLN. INFO.:			<u>JP 1999-20523</u>	A 19990128
			<u>JP 1999-283163</u>	A 19991004
			<u>WO 2000-JP444</u>	W 20000128

OTHER SOURCE(S): MARPAT 133:150920  
 GI



AB Substituted phenethylamine derivs. represented by general formula (I), hydrates of the same, or pharmaceutically acceptable salts thereof [wherein Cy is a group represented by general formula Q, an optionally substituted heterocyclic group, C3-7 cycloalkyl, or phenyl; R1, R1, R1, R1

and R5 are each hydrogen, halogeno, hydroxyl, amino, trifluoromethyl or cyano, at least one of R1-R5 being halogeno, trifluoromethyl or cyano; R6 represents hydrogen, (un)substituted linear or branched C1-3 alkyl, amino, or hydroxy; R8 represents hydrogen, Me, or ethyl; R9 represents (un)substituted linear or branched C1-6 alkyl, C2-6 alkenyl, or C2-6 alkynyl, C3-7 cycloalkyl, or (un)substituted Ph; R20 represents hydrogen, or (un)substituted linear or branched C1-3 alkyl or R9 and R20 together forms C3-7 cycloalkyl; R10 represents hydrogen, (un)substituted linear or branched C1-3 alkyl; R11 represents hydrogen or (un)substituted linear or branched C1-3 alkyl, (un)substituted carbamoyl, or carboxy; R12 represents hydroxy or linear or branched C1-4 alkoxy; R13 represents hydrogen, (un)substituted linear or branched C1-6 alkyl, C2-6 alkenyl, or alkynyl, etc.; X, Y represents carbonyl or CH2; provisos are given.], which exhibit motilin receptor antagonism and being useful as drugs for preventing digestive tract movement or high level of blood motilin. Thus, 3-methyl-2-methylaminobutyric acid 2-(3-tert-butyl-4-hydroxyphenyl)-1-(2-pyridylcarbamoyl)ethylamide (prepn. given) was condensed with Boc-Phe(4-F)-OH using CMPI in the presence of Et3N in THF under ice-cooling for 4 h followed by treatment of the product with CF3CO2H in CH2Cl2 gave 2-((2-amino-3-(4-fluorophenyl)propanoyl)-N-methylamino)-3-methylbutyric acid 2-(3-tert-butyl-4-hydroxyphenyl)-1-(2-pyridylcarbamoyl)ethylamide (II). II and N-Et-Phe(4-F)-N-Me-Val-N-Et-Tyr(3-tBu)-NHet showed IC50 of 0.35 and 0.17 nM, resp., for inhibiting binding of 125I-motilin to motilin receptor prepn. from mucus membrane of rabbit duodenum.

IT 287207-09-4P

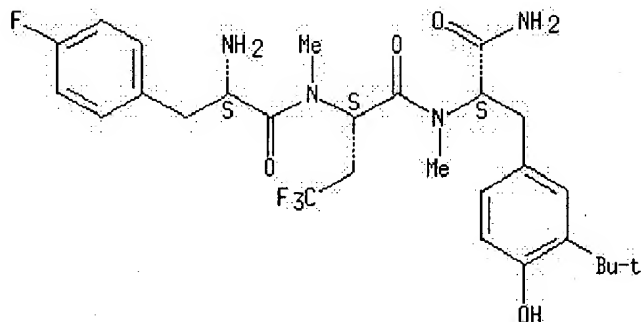
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of peptides or analogs contg. substituted phenethylamine moiety as motilin receptor antagonists and drugs for preventing digestive tract movement or high level of blood motilin)

RN 287207-09-4 HCAPLUS

CN L-Tyrosinamide, 4-fluoro-L-phenylalanyl-(2S)-4,4,4-trifluoro-2-(methylamino)butanoyl-3-(1,1-dimethylethyl)-N $\alpha$ -methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

41

THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold

COST IN U.S. DOLLARS

SINCE FILE ENTRY	TOTAL SESSION
7.12	2622.41

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.70	-7.70

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FILE COVERS 1907-1966  
 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d his

(FILE 'HOME' ENTERED AT 21:22:36 ON 02 SEP 2004)

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 L3 196 S L1 FULL

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 S L4

FILE 'REGISTRY' ENTERED AT 21:28:05 ON 02 SEP 2004

L5 1 S L4

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L6 1 S L5

FILE 'REGISTRY' ENTERED AT 21:28:09 ON 02 SEP 2004

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 L8 1 S L7

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L9 4 S L3

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 L13 352 S L11 FULL

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 L15 3 S L14 NOT L9



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L18 1 S L17 AND SATO, T?/AU  
L19 1 S L17 NOT L18  
L20 0 S L19 AND TAKAHASHI, T?/AU  
L21 0 S L17 AND KIM, D?/AU  
L22 0 S L17 AND JUNG, K?/AU  
L23 0 S L17 AND PARK, C?/AU  
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=> s 197

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COST IN U.S. DOLLARS

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TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

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TOTAL

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STRUCTURE FILE UPDATES: 1 SEP 2004 HIGHEST RN 737690-81-2

DICTIONARY FILE UPDATES: 1 SEP 2004 HIGHEST RN 737690-81-2

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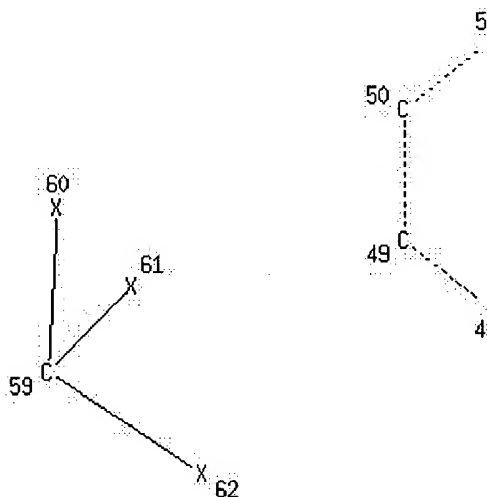
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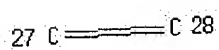
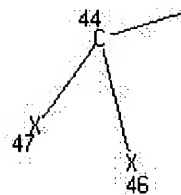
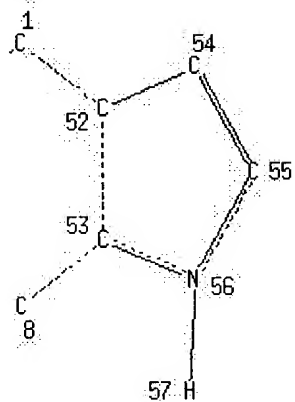
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Page 1-E



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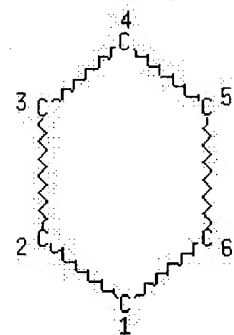
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Page 2-A



Page 2-B



Page 2-D

29 C  $\equiv$  C 30

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G11

7 C

G12 63

Page 2-E

37  
O  
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36

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C  
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018  
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017  
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14 C M2

Page 2-F

32

Page 3-A

26 G5

N 25

Page 3-D

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Page 3-E

G7

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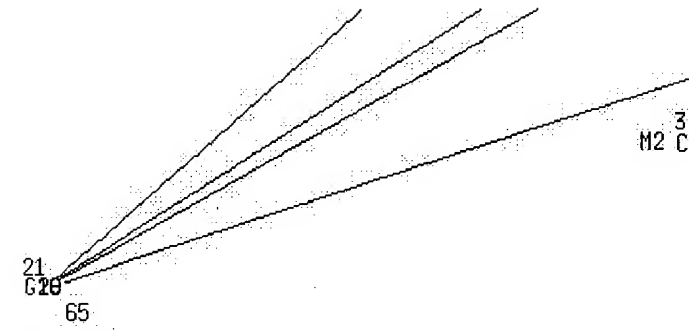
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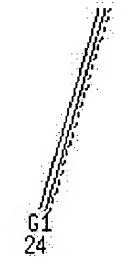
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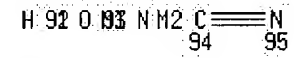
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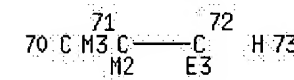
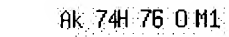
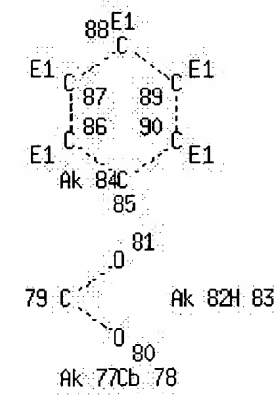
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Page 4-F



Page 8-D



Page 9-D

H 68 Ak 69

Page 10-D

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 VAR G5=74/75/76/25  
 VAR G6=77/78/27/29  
 VAR G7=79/82/83/23  
 VAR G8=33-10 33-12/34-10 34-12/36-10 36-12/38-10 38-12  
 VAR G9=84/85  
 VAR G11=6/54  
 VAR G12=91/92/93/94/59  
 REP G19=(1-2) 64-8 64-9  
 REP G20=(1-2) 14-13 14-16  
 VPA 22-18/19/20 S  
 VPA 31-17/18/19/20 S

NODE ATTRIBUTES:

HCOUNT	IS M2	AT	14
HCOUNT	IS M2	AT	33
HCOUNT	IS M2	AT	34
HCOUNT	IS M2	AT	35
HCOUNT	IS M2	AT	64
HCOUNT	IS M3	AT	70
HCOUNT	IS M2	AT	71
HCOUNT	IS E3	AT	72
HCOUNT	IS M1	AT	76
HCOUNT	IS E1	AT	86
HCOUNT	IS E1	AT	87
HCOUNT	IS E1	AT	88
HCOUNT	IS E1	AT	89
HCOUNT	IS E1	AT	90
HCOUNT	IS M1	AT	92
HCOUNT	IS M2	AT	93
NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS C	AT	7
NSPEC	IS C	AT	8
NSPEC	IS C	AT	9
NSPEC	IS C	AT	10
NSPEC	IS C	AT	11
NSPEC	IS C	AT	12
NSPEC	IS C	AT	13
NSPEC	IS C	AT	14
NSPEC	IS R	AT	15
NSPEC	IS R	AT	16
NSPEC	IS R	AT	17
NSPEC	IS R	AT	18
NSPEC	IS R	AT	19
NSPEC	IS R	AT	20
NSPEC	IS C	AT	21
NSPEC	IS C	AT	22
NSPEC	IS C	AT	23
NSPEC	IS C	AT	24
NSPEC	IS C	AT	25
NSPEC	IS C	AT	26
NSPEC	IS C	AT	27
NSPEC	IS C	AT	28
NSPEC	IS C	AT	29
NSPEC	IS C	AT	30
NSPEC	IS C	AT	31



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NSPEC  IS C      AT  32
NSPEC  IS C      AT  33
NSPEC  IS C      AT  34
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NSPEC  IS C      AT  37
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NSPEC  IS C      AT  45
NSPEC  IS C      AT  46
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NSPEC  IS R      AT  48
NSPEC  IS R      AT  49
NSPEC  IS R      AT  50
NSPEC  IS R      AT  51
NSPEC  IS R      AT  52
NSPEC  IS R      AT  53
NSPEC  IS R      AT  54
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NSPEC  IS R      AT  56
NSPEC  IS C      AT  57
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NSPEC  IS C      AT  61
NSPEC  IS C      AT  62
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NSPEC  IS C      AT  64
NSPEC  IS C      AT  65

```

DEFAULT MLEVEL IS ATOM

```

MLEVEL  IS CLASS AT   7  8  9 10 12 13 14 22 23 25 27 28 29 30 33 34 35
        36 37 38 39 44 45 46 47 48 49 54 55 56 57 59 60 61 62 64 66 67
        68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88
        89 90 91 92 93 94 95

```

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 95

STEREO ATTRIBUTES: NONE

=> s 1100

SAMPLE SEARCH INITIATED 22:42:44 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 806 TO ITERATE

100.0% PROCESSED 806 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 14417 TO 17823

PROJECTED ANSWERS: 0 TO 0

L101            0 SEA SSS SAM L100

=> s 1100 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:Y

FULL SEARCH INITIATED 22:42:53 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 16732 TO ITERATE

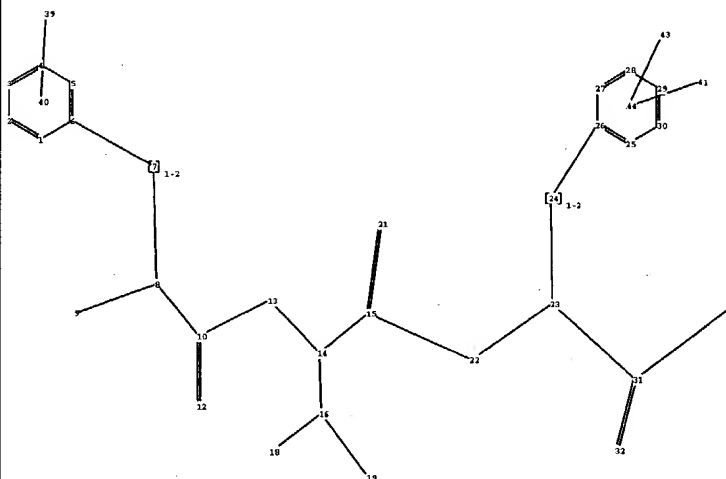
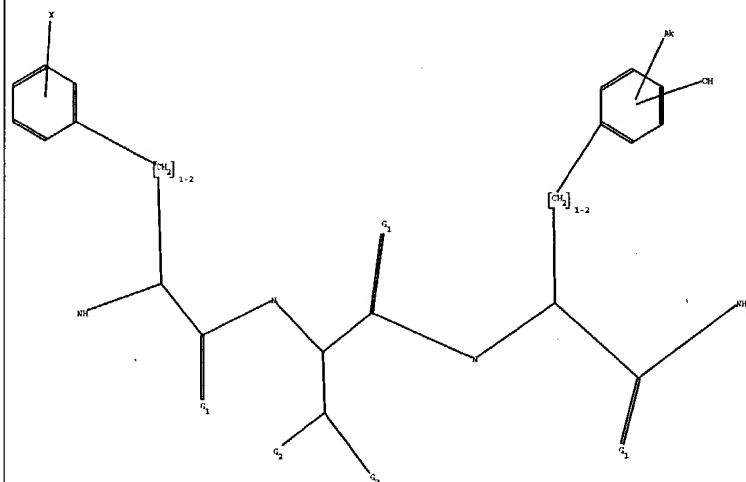
100.0% PROCESSED    16732 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L102            0 SEA SSS FUL L100

=>



chain nodes :

7 8 9 10 12 13 14 15 16 18 19 21 22 23 24 31 32 33 39 41 43

ring nodes :

1 2 3 4 5 6 25 26 27 28 29 30

chain bonds :

6-7 7-8 8-9 8-10 10-12 10-13 13-14 14-15 14-16 15-21 15-22 16-19 16-18 22-23  
23-24 23-31 24-26 31-32 31-33

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30

exact/norm bonds :

8-9 10-12 10-13 13-14 15-21 15-22 16-19 16-18 22-23 31-32 31-33

exact bonds :

6-7 7-8 8-10 14-15 14-16 23-24 23-31 24-26

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30

isolated ring systems :

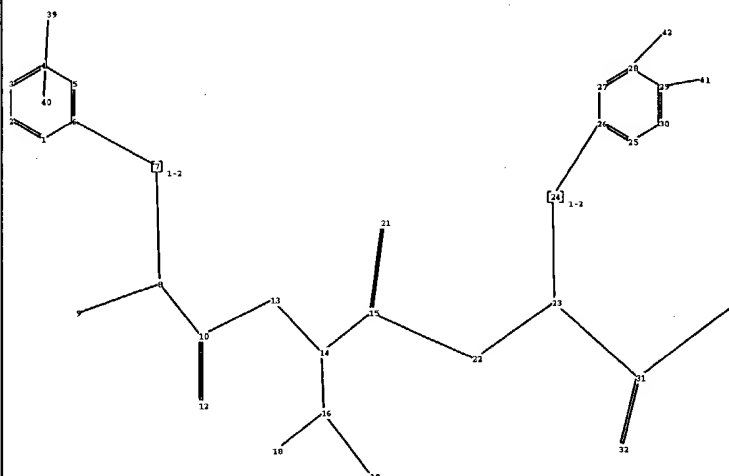
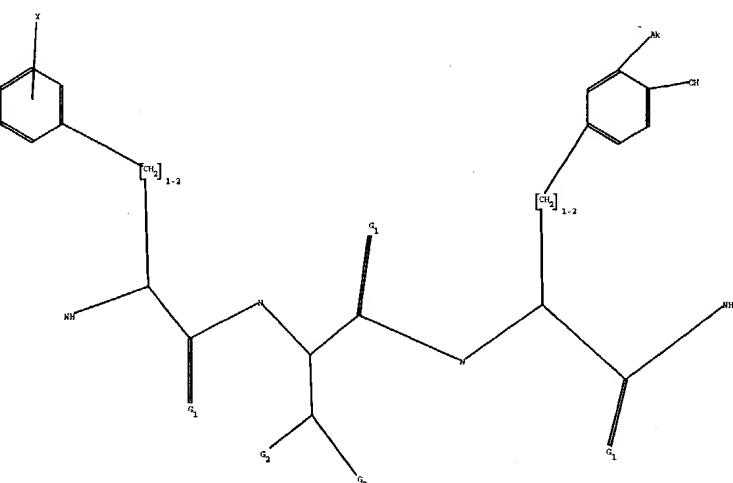
containing 1 : 25 :

G1:O,S

G2:CH3,Et

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS  
 23:CLASS 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS  
 32:CLASS 33:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS



chain nodes :

7 8 9 10 12 13 14 15 16 18 19 21 22 23 24 31 32 33 39 41 42

ring nodes :

1 2 3 4 5 6 25 26 27 28 29 30

chain bonds :

6-7 7-8 8-9 8-10 10-12 10-13 13-14 14-15 14-16 15-21 15-22 16-19 16-18 22-23  
23-24 23-31 24-26 28-42 29-41 31-32 31-33

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30

exact/norm bonds :

8-9 10-12 10-13 13-14 15-21 15-22 16-19 16-18 22-23 28-42 29-41 31-32 31-33

exact bonds :

6-7 7-8 8-10 14-15 14-16 23-24 23-31 24-26

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30

isolated ring systems :

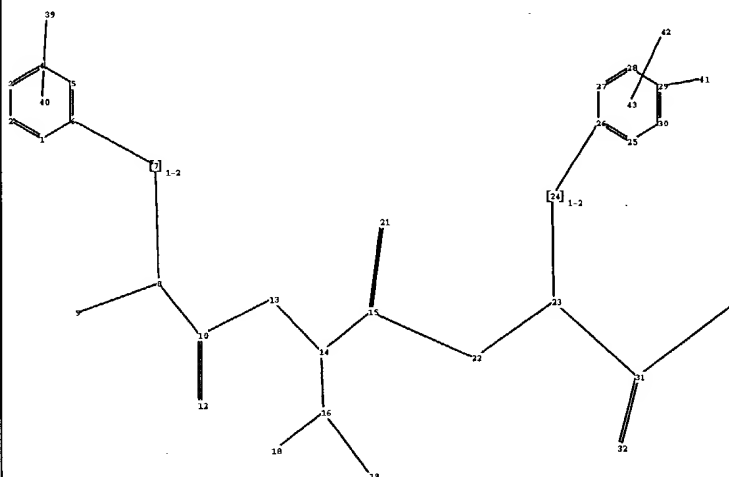
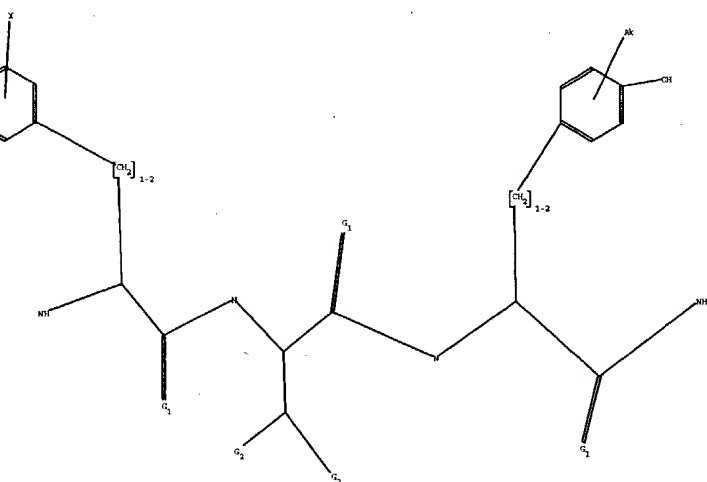
containing 1 : 25 :

G1:O,S

G2:CH3,Et

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS  
23:CLASS 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS  
32:CLASS 33:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS



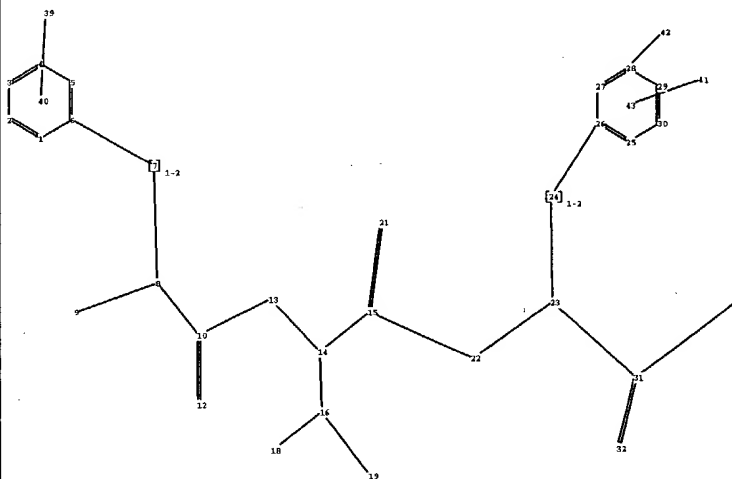
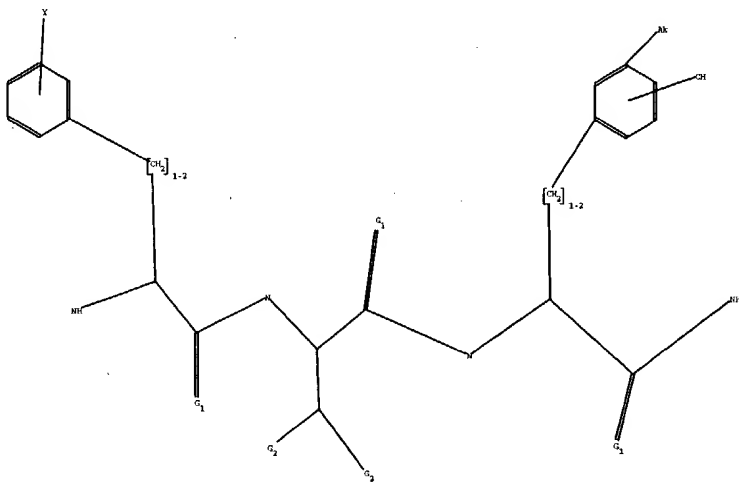
main nodes :  
 7 8 9 10 12 13 14 15 16 18 19 21 22 23 24 31 32 33 39 41 42  
 ng nodes :  
 1 2 3 4 5 6 25 26 27 28 29 30  
 ain bonds :  
 6-7 7-8 8-9 8-10 10-12 10-13 13-14 14-15 14-16 15-21 15-22 16-19 16-18 22-23  
 23-24 23-31 24-26 29-41 31-32 31-33  
 ng bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30  
 act/norm bonds :  
 8-9 10-12 10-13 13-14 15-21 15-22 16-19 16-18 22-23 29-41 31-32 31-33  
 act bonds :  
 6-7 7-8 8-10 14-15 14-16 23-24 23-31 24-26  
 rmalized bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30  
 olated ring systems :  
 containing 1 : 25 :

:O,S

:CH3,Et

atch level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS  
 23:CLASS 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS  
 32:CLASS 33:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS



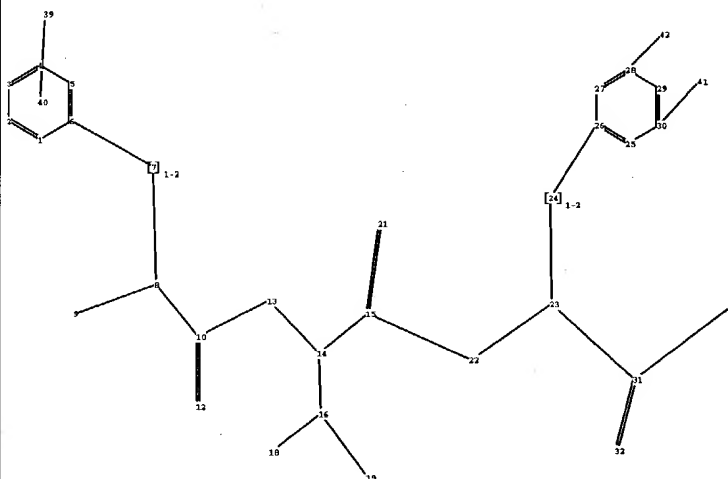
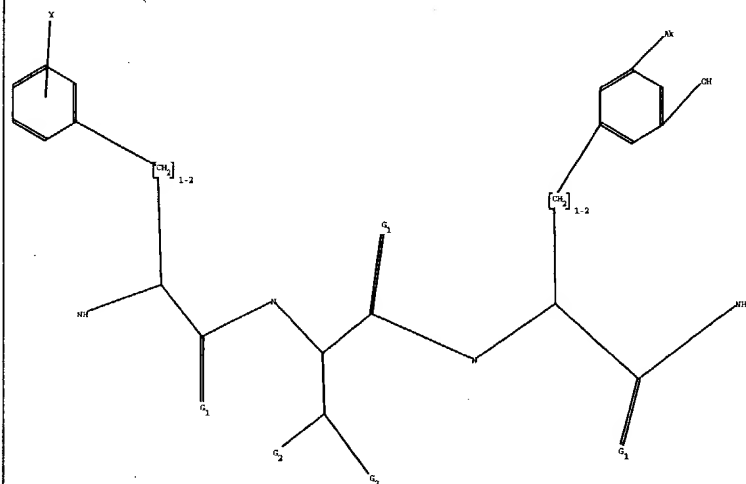
chain nodes :  
7 8 9 10 12 13 14 15 16 18 19 21 22 23 24 31 32 33 39 41 42  
ring nodes :  
1 2 3 4 5 6 25 26 27 28 29 30  
chain bonds :  
6-7 7-8 8-9 8-10 10-12 10-13 13-14 14-15 14-16 15-21 15-22 16-19 16-18 22-23  
23-24 23-31 24-26 28-42 31-32 31-33  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30  
exact/norm bonds :  
8-9 10-12 10-13 13-14 15-21 15-22 16-19 16-18 22-23 28-42 31-32 31-33  
exact bonds :  
6-7 7-8 8-10 14-15 14-16 23-24 23-31 24-26  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30  
isolated ring systems :  
containing 1 : 25 :

G1:O,S

G2:CH3,Et

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS  
23:CLASS 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS  
32:CLASS 33:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS

C:\stnweb\Queries\9a.str



chain nodes :

7 8 9 10 12 13 14 15 16 18 19 21 22 23 24 31 32 33 39 41 42

ring nodes :

1 2 3 4 5 6 25 26 27 28 29 30

chain bonds :

6-7 7-8 8-9 8-10 10-12 10-13 13-14 14-15 14-16 15-21 15-22 16-19 16-18 22-23  
23-24 23-31 24-26 28-42 30-41 31-32 31-33

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30

exact/norm bonds :

8-9 10-12 10-13 13-14 15-21 15-22 16-19 16-18 22-23 28-42 30-41 31-32 31-33

exact bonds :

6-7 7-8 8-10 14-15 14-16 23-24 23-31 24-26

normalized bonds :

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isolated ring systems :

containing 1 : 25 :

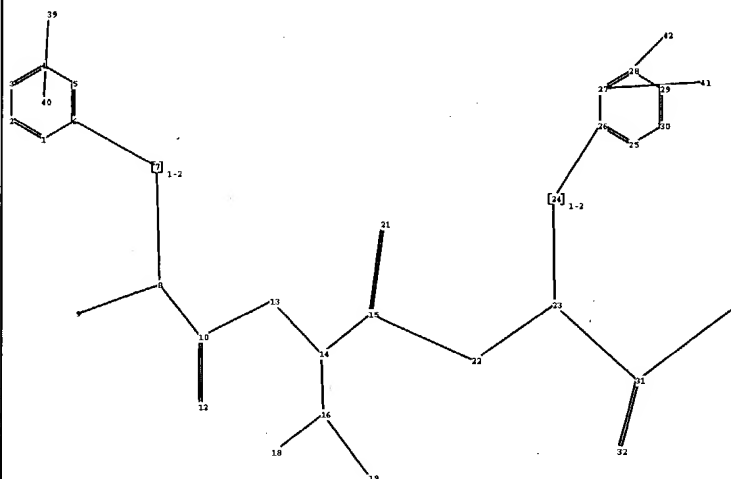
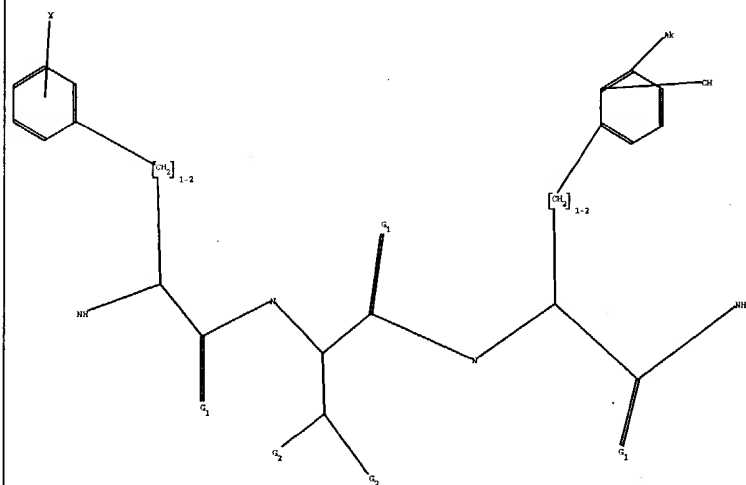
G1:O,S

G2:CH3,Et

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS  
23:CLASS 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS  
32:CLASS 33:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS

C:\stnweb\queries\4.str



chain nodes :

7 8 9 10 12 13 14 15 16 18 19 21 22 23 24 31 32 33 39 41 42

ring nodes :

1 2 3 4 5 6 25 26 27 28 29 30

chain bonds :

6-7 7-8 8-9 8-10 10-12 10-13 13-14 14-15 14-16 15-21 15-22 16-19 16-18 22-23  
23-24 23-31 24-26 27-41 28-42 31-32 31-33

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30

exact/norm bonds :

8-9 10-12 10-13 13-14 15-21 15-22 16-19 16-18 22-23 27-41 28-42 31-32 31-33

exact bonds :

6-7 7-8 8-10 14-15 14-16 23-24 23-31 24-26

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30

isolated ring systems :

containing 1 : 25 :

G1:O,S

G2:CH3,Et

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS  
23:CLASS 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS  
32:CLASS 33:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS



\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 "Ask CAS" for self-help around the clock  
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NEWS 4 May 12 Polymer links for the POLYLINK command completed in REGISTRY  
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NEWS 6 May 27 CAPLUS super roles and document types searchable in REGISTRY  
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NEWS 15 AUG 04 Pricing for the Save Answers for SciFinder Wizard within STN Express with Discover! will change September 1, 2004  
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NEWS 18 SEP 01 INPADOC: New family current-awareness alert (SDI) available  
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NEWS EXPRESS JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004  
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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 20:58:31 ON 02 SEP 2004

=> file req

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

h eb c g cg b cg

eb

FILE 'REGISTRY' ENTERED AT 20:58:58 ON 02 SEP 2004  
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provided by InfoChem.

STRUCTURE FILE UPDATES: 1 SEP 2004 HIGHEST RN 737690-81-2  
DICTIONARY FILE UPDATES: 1 SEP 2004 HIGHEST RN 737690-81-2

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR

=> s 1.1

SAMPLE SEARCH INITIATED 21:04:20 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 21339 TO ITERATE

4.7% PROCESSED 1000 ITERATIONS 1 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 418042 TO 435518  
PROJECTED ANSWERS: 149 TO 703

L2 1 SEA SSS SAM L1

=>

L3 STRUCTURE UPLOADED

=> d 13

L3 HAS NO ANSWERS

L3 STR

=> s 1.3

SAMPLE SEARCH INITIATED 21:05:37 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 11723 TO ITERATE

8.5% PROCESSED 1000 ITERATIONS 1 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 227975 TO 240945  
 PROJECTED ANSWERS: 29 TO 439

L4 1 SEA SSS SAM L3

=> s 13 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS  
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
 FULL SEARCH INITIATED 21:05:41 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 236139 TO ITERATE

100.0% PROCESSED 236139 ITERATIONS 128 ANSWERS  
 SEARCH TIME: 00.00.11

L5 128 SEA SSS FUL L3

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	160.04	160.25

FILE 'HCAPLUS' ENTERED AT 21:05:55 ON 02 SEP 2004  
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FILE COVERS 1907 - 2 Sep 2004 VOL 141 ISS 10  
 FILE LAST UPDATED: 1 Sep 2004 (20040901/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 15

L6 3 L5

=> s 16 and matsuoka, h?/au

2095 MATSUOKA, H?/AU

L7 1 L6 AND MATSUOKA, H?/AU

=> d 17, ibib abs fhitscr, 1

L7 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

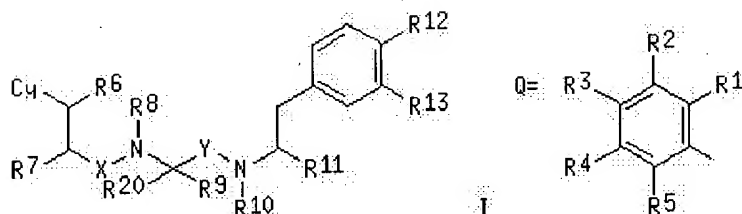
Full Text  CAS

ACCESSION NUMBER: 2000:535162 HCAPLUS

DOCUMENT NUMBER: 133:150920  
 TITLE: Preparation of peptides or analogs containing substituted phenethylamine moiety as motilin receptor antagonists  
 INVENTOR(S): **Matsuoka, Hiroharu**; Sato, Tsutomu; Takahashi, Tadakatsu; Kim, Dong Ick; Jung, Kyung Yun; Park, Chan Hee  
 PATENT ASSIGNEE(S): Chugai Seiyaku Kabushiki Kaisha, Japan  
 SOURCE: PCT Int. Appl., 403 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<u>WO 2000044770</u>	A1	20000803	<u>WO 2000-JP444</u>	20000128
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
<u>CA 2359030</u>	AA	20000803	<u>CA 2000-2359030</u>	20000128
<u>EP 1149843</u>	A1	20011031	<u>EP 2000-901956</u>	20000128
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
<u>NO 2001003684</u>	A	20010928	<u>NO 2001-3684</u>	20010726
<u>PRIORITY APPLN. INFO.:</u>			<u>JP 1999-20523</u>	A 19990128
			<u>JP 1999-283163</u>	A 19991004
			<u>WO 2000-JP444</u>	W 20000128

OTHER SOURCE(S): MARPAT 133:150920  
 GI



AB Substituted phenethylamine derivs. represented by general formula (I), hydrates of the same, or pharmaceutically acceptable salts thereof [wherein Cy is a group represented by general formula Q, an optionally substituted heterocyclic group, C3-7 cycloalkyl, or phenyl; R1, R1, R1, R1 and R5 are each hydrogen, halogeno, hydroxyl, amino, trifluoromethyl or cyano, at least one of R1-R5 being halogeno, trifluoromethyl or cyano; R6 represents hydrogen, (un)substituted linear or branched C1-3 alkyl, amino, or hydroxy; R8 represents hydrogen, Me, or ethyl; R9 represents (un)substituted linear or branched C1-6 alkyl, C2-6 alkenyl, or C2-6 alkynyl, C3-7 cycloalkyl, or (un)substituted Ph; R20 represents hydrogen, or (un)substituted linear or branched C1-3 alkyl or R9 and R20 together forms C3-7 cycloalkyl; R10 represents hydrogen, (un)substituted linear or

branched C1-3 alkyl; R11 represents hydrogen or (un)substituted linear or branched C1-3 alkyl, (un)substituted carbamoyl, or carboxy; R12 represents hydroxy or linear or branched C1-4 alkoxy; R13 represents hydrogen, (un)substituted linear or branched C1-6 alkyl, C2-6 alkenyl, or alkynyl, etc.; X, Y represents carbonyl or CH<sub>2</sub>; provisos are given.], which exhibit motilin receptor antagonism and being useful as drugs for preventing digestive tract movement or high level of blood motilin. Thus, 3-methyl-2-methylaminobutyric acid 2-(3-tert-butyl-4-hydroxyphenyl)-1-(2-pyridylcarbamoyl)ethylamide (prepn. given) was condensed with Boc-Phe(4-F)-OH using CMPI in the presence of Et<sub>3</sub>N in THF under ice-cooling for 4 h followed by treatment of the product with CF<sub>3</sub>CO<sub>2</sub>H in CH<sub>2</sub>Cl<sub>2</sub> gave 2-((2-amino-3-(4-fluorophenyl)propanoyl)-N-methylamino)-3-methylbutyric acid 2-(3-tert-butyl-4-hydroxyphenyl)-1-(2-pyridylcarbamoyl)ethylamide (II). II and N-Et-Phe(4-F)-N-Me-Val-N-Et-Tyr(3-tBu)-NH<sub>2</sub> showed IC<sub>50</sub> of 0.35 and 0.17 nM, resp., for inhibiting binding of <sup>125</sup>I-motilin to motilin receptor prep. from mucus membrane of rabbit duodenum.

IT **287205-81-6P**

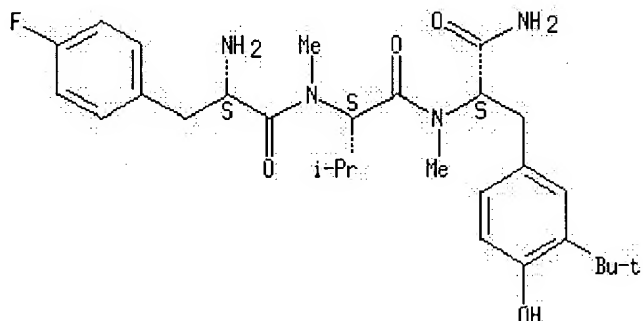
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of peptides or analogs contg. substituted phenethylamine moiety as motilin receptor antagonists and drugs for preventing digestive tract movement or high level of blood motilin)

RN **287205-81-6** HCAPLUS

CN L-Tyrosinamide, 4-fluoro-L-phenylalanyl-N-methyl-L-valyl-3-(1,1-dimethylethyl)-N-α-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 20:58:31 ON 02 SEP 2004)

FILE 'REGISTRY' ENTERED AT 20:58:58 ON 02 SEP 2004

L1 STRUCTURE UPLOADED  
L2 1 S L1  
L3 STRUCTURE UPLOADED  
L4 1 S L3  
L5 128 S L3 FULL

FILE 'HCAPLUS' ENTERED AT 21:05:55 ON 02 SEP 2004

L6 3 S L5  
L7 1 S L6 AND MATSUOKA, 'H?/AU

=&gt; s 16 not 17

L8 2 L6 NOT L7

=&gt; s 18 and sato, t?/au

20671 SATO, T?/AU

L9 1 L8 AND SATO, T?/AU

=&gt; d 19, ibib abs fhitstr, 1

L9 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	References
--------------	------------

ACCESSION NUMBER: 2002:90066 HCAPLUS  
DOCUMENT NUMBER: 136:135034  
TITLE: Method for producing tripeptide derivative  
INVENTOR(S): Sato, Tsutomu; Shimizu, Hirohito  
PATENT ASSIGNEE(S): Chugai Seiyaku Kabushiki Kaisha, Japan  
SOURCE: PCT Int. Appl., 50 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002008248	A1	20020131	WO 2001-JP6295	20010719
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.:			JP 2000-219977	A 20000721
OTHER SOURCE(S):			CASREACT 136:135034; MARPAT 136:135034	
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB A method for producing L-phenylalanyl-L-valyl-L-3-tert-butyl-L-tyrosinamide compds. represented by the general formula (I; wherein R1 represents a hydrogen atom or a linear or branched aliph. alkyl group having 1 to 4 carbon atoms; R2 represents a hydrogen atom or Me group; R3 represents a hydrogen atom or Me group; and R4 represents a halogen atom) comprises condensation of 3-tert-butyl-L-tyrosinamide derivs. (II; R1, R2 = same as above) with N-methyl-L-valine derivs. (III; P1 = amino-protecting group), N-deprotection of the resulting L-valyl-3-tert-butyl-L-tyrosinamide derivs. (IV; R1, R2, P1 = same as above), and condensation of the resulting IV (P1 = H; R1, R2 = same as above) with L-phenylalanine derivs. (V; R3, R4 = same as above; P2 = amino-protecting group) followed by N-deprotection. The method can be advantageously used for producing a novel peptide deriv. in a com. process. Thus, 20.8 g MeSO3H and 20.0 g tert-Bu chloride were

successively added to 10.0 g L-tyrosine Me ester hydrochloride under stirring, stirred at 50° for 5 h, treated dropwise with MeOH (20 mL)/H<sub>2</sub>O (20 mL) under ice-cooling then with a soln. of 14.2 g KOH in 43 mL H<sub>2</sub>O at <10° to give 77.0% 3-tert-butyl-L-tyrosine Me ester which (8.35 g) was added to a mixt. of 24.1 g 62% aq. ethylamine and 7.52 g ethylamine hydrochloride under ice-cooling and stirred at room temp. for 5 h to give 89.8% 3-tert-butyl-L-tyrosine ethylamide (VI). To a soln. of 5.50 g VI and 3.35 g 1-hydroxybenzotriazole monohydrate in 55 mL THF were successively added 4.19 g 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride and 3.04 mL Et<sub>3</sub>N and stirred at room temp. for 2.5 h to give 100% N-tert-butoxycarbonyl-N-methyl-L-valyl-3-tert-butyl-L-tyrosine ethylamide which (10.0 g) was dissolved in 100 mL EtOAc, treated with 11.1 mL concd. H<sub>2</sub>SO<sub>4</sub> under ice-cooling, treated with 100 mL EtOAc, adjusted pH 8 by adding satd. aq. NaHCO<sub>3</sub>, and stirred 15 min to give 87.9% N-methyl-L-valyl-3-tert-butyl-L-tyrosine ethylamide (VII). To a mixt. of 5.50 g VII, 5.20 g N-tert-butoxycarbonyl-N-methyl-4-fluoro-L-phenylalanine, 4.47 g 2-chloro-1-methylpyridinium iodide, and 37 mL tert-Bu Me ether was added 5.09 mL Et<sub>3</sub>N and stirred at room temp. for 4 h to give 86.0% N-tert-butoxycarbonyl-N-methyl-4-fluoro-L-phenylalanyl-N-methyl-L-valyl-3-tert-butyl-L-tyrosine ethylamide which (7.50 g) was similarly deprotected as described above using concd. H<sub>2</sub>SO<sub>4</sub> in EtOAc to give 100% N-methyl-4-fluoro-L-phenylalanyl-N-methyl-L-valyl-3-tert-butyl-L-tyrosine.

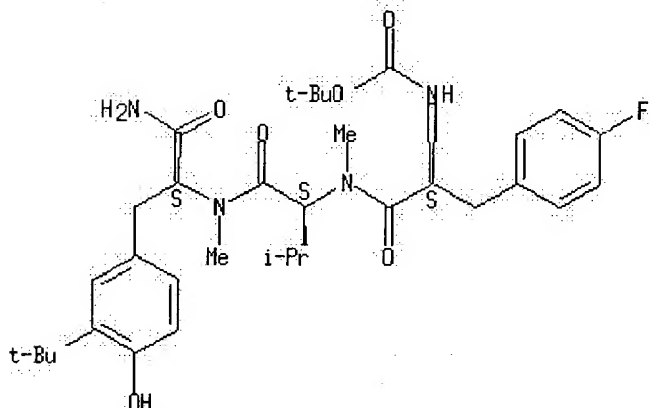
IT **393562-03-3P**

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. tripeptide derivs. by sequential coupling of N-methyl-L-valine derivs. and L-phenylalanine derivs. to 3-tert-butyl-L-tyrosinamide derivs.)

RN **393562-03-3** HCAPLUS

CN L-Tyrosinamide, N-[(1,1-dimethylethoxy)carbonyl]-4-fluoro-L-phenylalanyl-N-methyl-L-valyl-3-(1,1-dimethylethyl)-N- $\alpha$ -methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

7

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=&gt; d his

(FILE 'HOME' ENTERED AT 20:58:31 ON 02 SEP 2004)

FILE 'REGISTRY' ENTERED AT 20:58:58 ON 02 SEP 2004

L1 STRUCTURE UPLOADED

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L2 1 S L1  
 L3 STRUCTURE UPLOADED  
 L4 1 S L3  
 L5 128 S L3 FULL

FILE 'HCAPLUS' ENTERED AT 21:05:55 ON 02 SEP 2004

L6 3 S L5  
 L7 1 S L6 AND MATSUOKA, H?/AU  
 L8 2 S L6 NOT L7  
 L9 1 S L8 AND SATO, T?/AU

=> s l8 not l9

L10 1 L8 NOT L9

=> s l10 and takahashi, t?/au  
 17491 TAKAHASHI, T?/AU

L11 0 L10 AND TAKAHASHI, T?/AU

=> s l10 and kim, d?/au  
 13514 KIM, D?/AU

L12 1 L10 AND KIM, D?/AU

=> d l2, ibib abs fhistr, 1

1 ANSWERS ARE AVAILABLE. SPECIFIED ANSWER NUMBER EXCEEDS ANSWER SET SIZE

The answer numbers requested are not in the answer set.

ENTER ANSWER NUMBER OR RANGE (1):0

NUMBERS IN RANGE MUST BE GREATER THAN ZERO.

An answer number must be a positive number.

ENTER ANSWER NUMBER OR RANGE (1):0

NUMBERS IN RANGE MUST BE GREATER THAN ZERO.

An answer number must be a positive number.

ENTER ANSWER NUMBER OR RANGE (1):1

L12 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

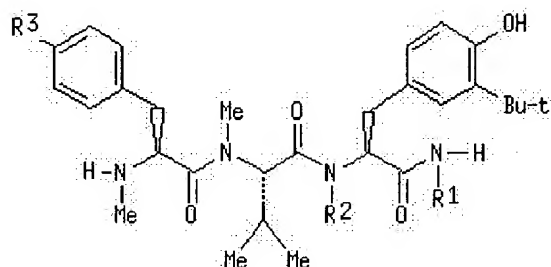
Full Text	Cite References
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ACCESSION NUMBER: 2002:637704 HCAPLUS  
 DOCUMENT NUMBER: 137:185838  
 TITLE: Process for preparation of peptide derivatives  
 INVENTOR(S): Kim, Dong Ick; Jeon, Gee Ho; Kim, Sung Jin  
 PATENT ASSIGNEE(S): Chugai Seiyaku Kabushiki Kaisha, Japan  
 SOURCE: PCT Int. Appl., 40 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002064623	A1	20020822	WO 2002-JP1139	20020212
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,				



BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG  
 PRIORITY APPLN. INFO.: KR 2001-6673 A 20010212  
 OTHER SOURCE(S): CASREACT 137:185838; MARPAT 137:185838  
 GI



I

AB The title compds. I [R1 is hydrogen or linear or branched C1-4 alkyl; R2 is hydrogen or linear or branched C1-4 alkyl; and R3 is halogeno] are prepd. in a multistep process. I are motilin receptor antagonists and are useful as drugs for gastric or intestinal diseases (no data). Thus, amidation of N-(tert-butoxycarbonyl)-L-(4-fluorophenyl)alanine with L-valine Me ester hydrochloride, followed by methylation with iodomethane, sapon., reaction with 3-tert-butyl-L-tyrosine Et amide, and deprotection, gave N-methyl-L-4-fluorophenylalanyl-N-methyl-L-valine-3-tert-butyl-L-tyrosine Et amide.

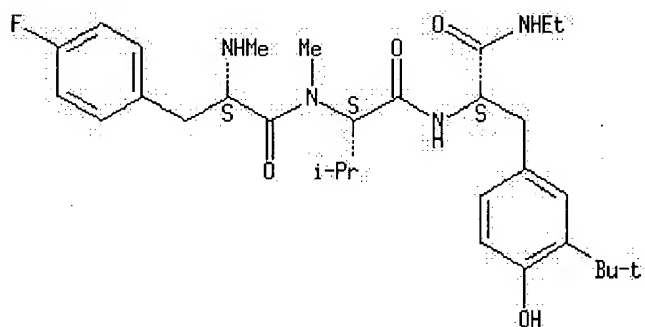
IT **287206-61-5P**

RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (process for prepn. of peptide derivs.)

RN 287206-61-5 HCAPLUS

CN L-Tyrosinamide, 4-fluoro-N-methyl-L-phenylalanyl-N-methyl-L-valyl-3-(1,1-dimethylethyl)-N-ethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 20:58:31 ON 02 SEP 2004)

FILE 'REGISTRY' ENTERED AT 20:58:58 ON 02 SEP 2004

L1 STRUCTURE UPLOADED

L2 1 S L1  
 L3 STRUCTURE UPLOADED  
 L4 1 S L3  
 L5 128 S L3 FULL

FILE 'HCAPLUS' ENTERED AT 21:05:55 ON 02 SEP 2004

L6 3 S L5  
 L7 1 S L6 AND MATSUOKA, H?/AU  
 L8 2 S L6 NOT L7  
 L9 1 S L8 AND SATO, T?/AU  
 L10 1 S L8 NOT L9  
 L11 0 S L10 AND TAKAHASHI, T?/AU  
 L12 1 S L10 AND KIM, D?/AU

=> d l12, ibib abs fhitstr, i

L12 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full  
 Text

ACCESSION NUMBER: 2002:637704 HCAPLUS  
 DOCUMENT NUMBER: 137:185838  
 TITLE: Process for preparation of peptide derivatives  
 INVENTOR(S): Kim, Dong Ick; Jeon, Gee Ho; Kim, Sung Jin  
 PATENT ASSIGNEE(S): Chugai Seiyaku Kabushiki Kaisha, Japan  
 SOURCE: PCT Int. Appl., 40 pp.  
 CODEN: PIXXD2

DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

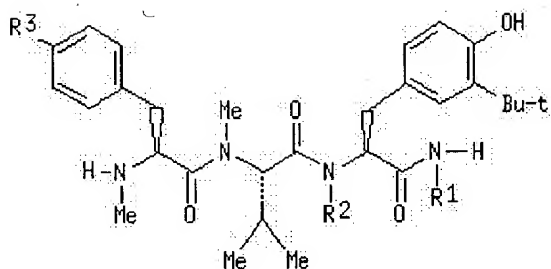
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002064623	A1	20020822	WO 2002-JP1139	20020212
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: KR 2001-6673 A 20010212

OTHER SOURCE(S): CASREACT 137:185838; MARPAT 137:185838

GI



I

AB The title compds. I [R1 is hydrogen or linear or branched C1-4 alkyl; R2 is hydrogen or linear or branched C1-4 alkyl; and R3 is halogeno] are prepd. in a multistep process. I are motilin receptor antagonists and are useful as drugs for gastric or intestinal diseases (no data). Thus, amidation of N-(tert-butoxycarbonyl)-L-(4-fluorophenyl)alanine with L-valine Me ester hydrochloride, followed by methylation with iodomethane, sapon., reaction with 3-tert-butyl-L-tyrosine Et amide, and deprotection, gave N-methyl-L-4-fluorophenylalanyl-N-methyl-L-valine-3-tert-butyl-L-tyrosine Et amide.

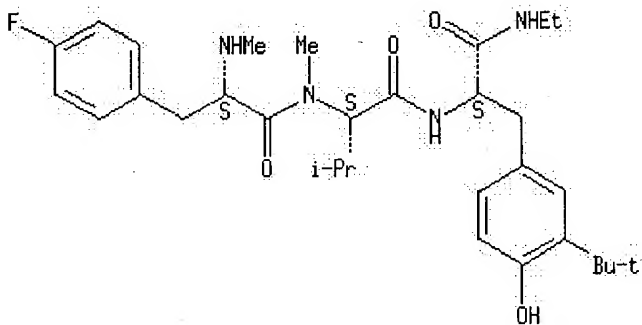
IT **287206-61-5P**

RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(process for prepn. of peptide derivs.)

RN 287206-61-5 HCAPLUS

CN L-Tyrosinamide, 4-fluoro-N-methyl-L-phenylalanyl-N-methyl-L-valyl-3-(1,1-dimethylethyl)-N-ethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold

COST IN U.S. DOLLARS

SINCE FILE ENTRY	TOTAL SESSION
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FULL ESTIMATED COST

28.48	188.73
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE ENTRY	TOTAL SESSION
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CA SUBSCRIBER PRICE

-2.80	-2.80
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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d his

(FILE 'HOME' ENTERED AT 20:58:31 ON 02 SEP 2004)

FILE 'REGISTRY' ENTERED AT 20:58:58 ON 02 SEP 2004

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 STRUCTURE UPLOADED

L4 1 S L3

L5 128 S L3 FULL

FILE 'HCAPLUS' ENTERED AT 21:05:55 ON 02 SEP 2004

L6 3 S L5

L7 1 S L6 AND MATSUOKA, H?/AU

L8 2 S L6 NOT L7

L9 1 S L8 AND SATO, T?/AU

L10 1 S L8 NOT L9

L11 0 S L10 AND TAKAHASHI, T?/AU

L12 1 S L10 AND KIM, D?/AU

FILE 'CAOLD' ENTERED AT 21:08:12 ON 02 SEP 2004

=> s l5

L13 0 L5

=> file reg

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 1 SEP 2004 HIGHEST RN 737690-81-2

DICTIONARY FILE UPDATES: 1 SEP 2004 HIGHEST RN 737690-81-2

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

L14 STRUCTURE UPLOADED

=> d l14

L14 HAS NO ANSWERS

L14 STR

=> s l14

SAMPLE SEARCH INITIATED 21:09:07 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 11723 TO ITERATE

8.5% PROCESSED 1000 ITERATIONS 1 ANSWERS  
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 227975 TO 240945

PROJECTED ANSWERS: 29 TO 439

L15 1 SEA SSS SAM L14

=> s l14 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 21:09:14 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 236139 TO ITERATE

100.0% PROCESSED 236139 ITERATIONS 128 ANSWERS  
 SEARCH TIME: 00.00.12

L16 128 SEA SSS FUL L14

=> d h1s

(FILE 'HOME' ENTERED AT 20:58:31 ON 02 SEP 2004)

FILE 'REGISTRY' ENTERED AT 20:58:58 ON 02 SEP 2004

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 STRUCTURE UPLOADED

L4 1 S L3

L5 128 S L3 FULL

FILE 'HCAPLUS' ENTERED AT 21:05:55 ON 02 SEP 2004

L6 3 S L5

L7 1 S L6 AND MATSUOKA, H?/AU

L8 2 S L6 NOT L7

L9 1 S L8 AND SATO, T?/AU

L10 1 S L8 NOT L9  
 L11 0 S L10 AND TAKAHASHI, T?/AU  
 L12 1 S L10 AND KIM, D?/AU

FILE 'CAOLD' ENTERED AT 21:08:12 ON 02 SEP 2004  
 L13 0 S L5

FILE 'REGISTRY' ENTERED AT 21:08:18 ON 02 SEP 2004  
 L14 STRUCTURE UPLOADED  
 L15 1 S L14  
 L16 128 S L14 FULL

=> s 116 not 15  
 L17 0 L16 NOT L5

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 L18 STRUCTURE UPLOADED

=> d 118  
 L18 HAS NO ANSWERS  
 L18 STR

=> s 118  
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 SAMPLE SCREEN SEARCH COMPLETED - 21339 TO ITERATE

4.7% PROCESSED 1000 ITERATIONS  
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
 SEARCH TIME: 00.00.01

1 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 418042 TO 435518  
 PROJECTED ANSWERS: 149 TO 703

L19 1 SEA SSS SAM L18

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 L20 STRUCTURE UPLOADED

=> d 120  
 L20 HAS NO ANSWERS  
 L20 STR

=> s 120  
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 SAMPLE SCREEN SEARCH COMPLETED - 21339 TO ITERATE

4.7% PROCESSED 1000 ITERATIONS  
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
 SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 418042 TO 435518  
 PROJECTED ANSWERS: 0 TO 0

L21 0 SEA SSS SAM L20

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L22        STRUCTURE UPLOADED

=> d 122

L22 HAS NO ANSWERS

L22                STR

=> s 122

SAMPLE SEARCH INITIATED 21:12:17 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED -        153 TO ITERATE

100.0% PROCESSED        153 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:    ONLINE    \*\*COMPLETE\*\*

BATCH    \*\*COMPLETE\*\*

PROJECTED ITERATIONS:        2318 TO        3802

PROJECTED ANSWERS:                0 TO        0

L23                0 SEA SSS SAM L22

=> s 122

SAMPLE SEARCH INITIATED 21:12:20 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED -        153 TO ITERATE

100.0% PROCESSED        153 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:    ONLINE    \*\*COMPLETE\*\*

BATCH    \*\*COMPLETE\*\*

PROJECTED ITERATIONS:        2318 TO        3802

PROJECTED ANSWERS:                0 TO        0

L24                0 SEA SSS SAM L22

=> s 122 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 21:12:26 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED -        2746 TO ITERATE

100.0% PROCESSED        2746 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L25                0 SEA SSS FUL L22

=>

L26        STRUCTURE UPLOADED

=> 126

L26 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.

For a list of commands available to you in the current file, enter

"HELP COMMANDS" at an arrow prompt (=>).

=> d 126

L26 HAS NO ANSWERS

L26                STR

=> s 126

SAMPLE SEARCH INITIATED 21:13:07 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 342 TO ITERATE

100.0% PROCESSED 342 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 5731 TO 7949  
PROJECTED ANSWERS: 0 TO 0

L27 0 SEA SSS SAM L26

=> s 126 full

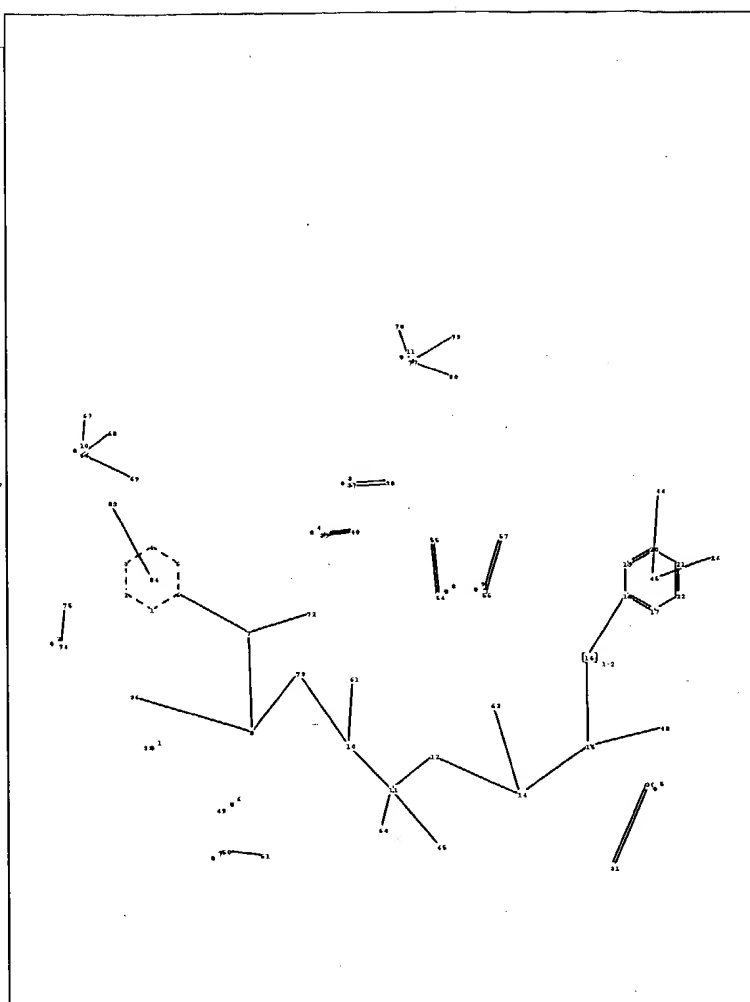
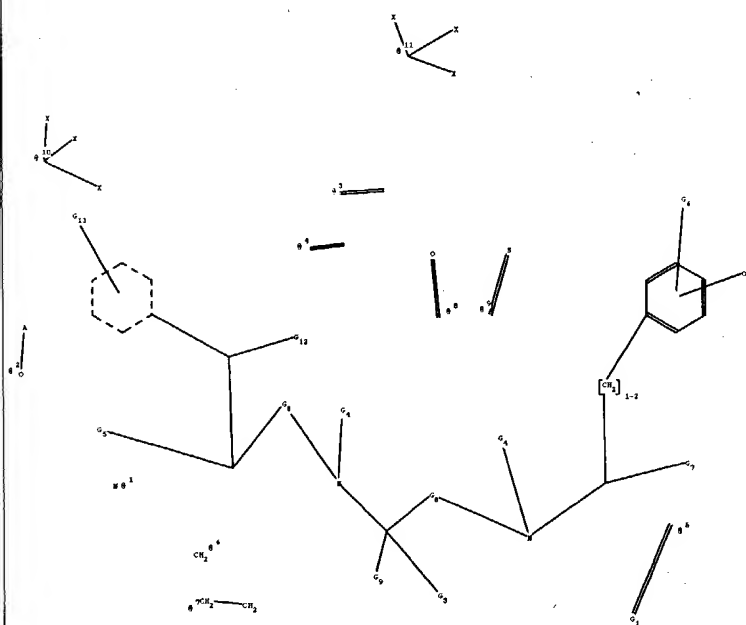
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
FULL SEARCH INITIATED 21:13:12 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 7164 TO ITERATE

100.0% PROCESSED 7164 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

L28 0 SEA SSS FUL L26

=>





chain nodes :

7 8 10 11 12 14 15 16 26 30 31 33 36 37 38 39 40 44 48 49 50 51 54  
55 56 57 61 62 64 65 66 67 68 69 72 73 74 75 77 78 79 80 83

ring nodes :

1 2 3 4 5 6 17 18 19 20 21 22

chain bonds :

6-7 7-8 7-72 8-36 8-73 10-61 10-11 10-73 11-12 11-64 11-65 12-14 14-15 14-62  
15-16 15-48 16-18 30-31 37-38 39-40 50-51 54-55 56-57 66-68 66-69 66-67 74-75  
77-79 77-80 77-78

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 17-18 17-22 18-19 19-20 20-21 21-22

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-72 8-36 10-61 10-11 11-12 11-64 11-65 12-14 14-15  
14-62 15-48 30-31 54-55 56-57 74-75

exact bonds :

6-7 7-8 8-73 10-73 15-16 16-18 37-38 39-40 50-51 66-68 66-69 66-67 77-79  
77-80 77-78

normalized bonds :

17-18 17-22 18-19 19-20 20-21 21-22

isolated ring systems :

containing 1 : 17 :

G1:O,S

G2:CH3,Et

G3:H,Ak

G4:CH3,Et,H

G5:Ak,H,OH,[\*1],[\*2]

G6:Ak,Cb,[\*3],[\*4]

G7:COOH,Ak,H,[\*5]

G8:[\*6],[\*7],[\*8],[\*9]

G9:Ak,Ph

G12:H,OH,NH2,CN,[\*10]

G13:CN,X,[\*11]

Match level :

1:Atom	2:Atom	3:Atom	4:Atom	5:Atom	6:Atom	7:CLASS	8:CLASS	10:CLASS	11:CLASS
12:CLASS	14:CLASS	15:CLASS	16:CLASS	17:Atom	18:Atom	19:Atom	20:Atom	21:Atom	
22:Atom	26:CLASS	27:CLASS	30:CLASS	31:CLASS	33:CLASS	36:CLASS	37:CLASS	38:CLASS	
39:CLASS	40:CLASS	44:CLASS	45:CLASS	48:CLASS	49:CLASS	50:CLASS	51:CLASS	54:CLASS	
55:CLASS	56:CLASS	57:CLASS	61:CLASS	62:CLASS	64:CLASS	65:CLASS	66:CLASS	67:CLASS	
68:CLASS	69:CLASS	72:CLASS	73:CLASS	74:CLASS	75:CLASS	77:CLASS	78:CLASS	79:CLASS	
80:CLASS	83:CLASS	84:CLASS							

=&gt;

L124        STRUCTURE UPLOADED

=&gt; d 1124

L124 HAS NO ANSWERS

L124                STR

=&gt; s 1124

SAMPLE SEARCH INITIATED 23:29:57 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 17092 TO ITERATE

5.9% PROCESSED        1000 ITERATIONS                                1 ANSWERS  
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:    ONLINE    \*\*COMPLETE\*\*  
                               BATCH    \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS:        334015 TO    349665  
 PROJECTED ANSWERS:                93 TO        589

L125                1 SEA SSS SAM L124

=&gt; s 1125

SAMPLE SEARCH INITIATED 23:30:08 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 17092 TO ITERATE

5.9% PROCESSED        1000 ITERATIONS                                1 ANSWERS  
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:    ONLINE    \*\*COMPLETE\*\*  
                               BATCH    \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS:        334015 TO    349665  
 PROJECTED ANSWERS:                93 TO        589

L126                1 SEA SSS SAM L124

=&gt; s 1125 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 23:30:49 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 342655 TO ITERATE

100.0% PROCESSED    342655 ITERATIONS                                353 ANSWERS  
 SEARCH TIME: 00.00.16

L127                353 SEA SSS FUL L124

=&gt; file hcaplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	329.32	3308.11

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-9.10

FILE 'HCAPLUS' ENTERED AT 23:31:50 ON 02 SEP 2004  
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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FILE COVERS 1907 - 2 Sep 2004 VOL 141 ISS 10

FILE LAST UPDATED: 1 Sep 2004 (20040901/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 1127

L128 4 L127

=> s 1128 and matsuoka, h?/au

2095 MATSUOKA, H?/AU

L129 2 L128 AND MATSUOKA, H?/AU

=> d 129, ibib abs fhitr, 1-2

L29 HAS NO ANSWERS

'IBIB ABS FHITSTR' IS NOT A VALID STRUCTURE FORMAT KEYWORD

Structure Formats

SIA ----- Structure Image, Attributes, and map table if it contains data. (Default)

SIM ----- Structure Image.

SAT ----- Structure ATtributes and map table if it contains data.

SCT ----- Structure Connection Table and map table if it contains data.

SDA ----- All Structure DATA (image, attributes, connection table and map table if it contains data).

NOS ----- NO Structure data.

ENTER STRUCTURE FORMAT (SIA), SCT, SDA, SIM, SAT, NOS:end

=> d 1129, ibib abs fhitr, 1-2

L129 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
--------------	----------------------

ACCESSION NUMBER: 2002:157810 HCAPLUS

DOCUMENT NUMBER: 136:217049

TITLE: Preparation of cyclic peptide derivatives as motilin receptor antagonists

INVENTOR(S): Matsuoka, Hiroharu; Sato, Tsutomu

PATENT ASSIGNEE(S): Chugai Seiyaku Kabushiki Kaisha, Japan

SOURCE: PCT Int. Appl., 89 pp.

CODEN: PIXXD2

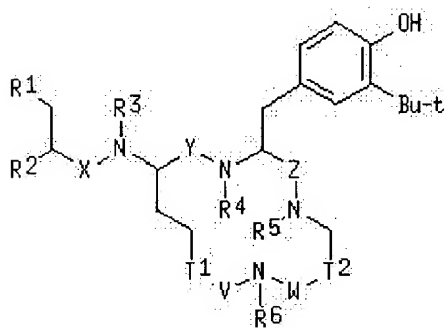
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<u>WO 2002016404</u>	A1	20020228	<u>WO 2001-JP7213</u>	20010823
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
<u>AU 2001080120</u>	A5	20020304	<u>AU 2001-80120</u>	20010823
<u>EP 1312612</u>	A1	20030521	<u>EP 2001-958426</u>	20010823
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
<u>US 2003191053</u>	A1	20031009	<u>US 2003-362574</u>	20030224
<u>PRIORITY APPLN. INFO.:</u>			<u>JP 2000-253950</u>	A 20000824
			<u>WO 2001-JP7213</u>	W 20010823
OTHER SOURCE(S):		MARPAT 136:217049		
GI				



I

AB The title compds. I [T1 = (CH<sub>2</sub>)<sub>m</sub>; T2 = (CH<sub>2</sub>)<sub>n</sub>; R1 represents optionally substituted Ph, etc.; R2 represents amino, etc.; R3 to R6 each represents hydrogen, Me, etc.; V, W, X, Y, Z represent carbonyl or methylene; m is an integer of 0 to 2; and n is an integer of 0 to 3] are prepd. In an in vitro test for motilin receptor antagonism, (2S-(2S,12S))-2-amino-N-(2-(3-tert-butyl-4-hydroxyphenylmethyl)-1,4,8-triaza-3,7,13-trioxocyclotridecan-12-yl)-3-(4-fluorophenyl)-N-methylpropionamide showed IC<sub>50</sub> of 0.52 nM.

IT 401896-13-7P

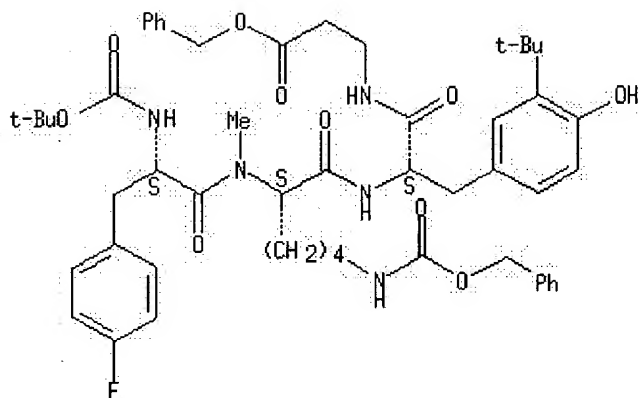
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of cyclic peptide derivs. as motilin receptor antagonists)

RN 401896-13-7 HCAPLUS

CN β-Alanine, N-[(1,1-dimethylethoxy)carbonyl]-4-fluoro-L-phenylalanyl-N2-methyl-N6-[(phenylmethoxy)carbonyl]-L-lysyl-3-(1,1-dimethylethyl)-L-tyrosyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



*Claims*  
19

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

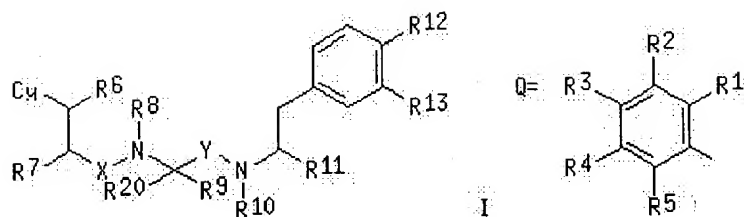
L129 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text  
Chemical Structures

ACCESSION NUMBER: 2000:535162 HCAPLUS  
DOCUMENT NUMBER: 133:150920  
TITLE: Preparation of peptides or analogs containing substituted phenethylamine moiety as motilin receptor antagonists  
INVENTOR(S): Matsuoka, Hiroharu; Sato, Tsutomu; Takahashi, Tadakatsu; Kim, Dong Ick; Jung, Kyung Yun; Park, Chan Hee  
PATENT ASSIGNEE(S): Chugai Seiyaku Kabushiki Kaisha, Japan  
SOURCE: PCT Int. Appl., 403 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<u>WO 2000044770</u>	A1	20000803	<u>WO 2000-JP444</u>	20000128
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
<u>CA 2359030</u>	AA	20000803	<u>CA 2000-2359030</u>	20000128
<u>EP 1149843</u>	A1	20011031	<u>EP 2000-901956</u>	20000128
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
<u>NO 2001003684</u>	A	20010928	<u>NO 2001-3684</u>	20010726
PRIORITY APPLN. INFO.:				
			<u>JP 1999-20523</u>	A 19990128
			<u>JP 1999-283163</u>	A 19991004
			<u>WO 2000-JP444</u>	W 20000128

OTHER SOURCE(S): MARPAT 133:150920  
GI



AB Substituted phenethylamine derivs. represented by general formula (I), hydrates of the same, or pharmaceutically acceptable salts thereof [wherein Cy is a group represented by general formula Q, an optionally substituted heterocyclic group, C3-7 cycloalkyl, or phenyl; R1, R1, R1, R1 and R5 are each hydrogen, halogeno, hydroxyl, amino, trifluoromethyl or cyano, at least one of R1-R5 being halogeno, trifluoromethyl or cyano; R6 represents hydrogen, (un)substituted linear or branched C1-3 alkyl, amino, or hydroxy; R8 represents hydrogen, Me, or ethyl; R9 represents (un)substituted linear or branched C1-6 alkyl, C2-6 alkenyl, or C2-6 alkynyl, C3-7 cycloalkyl, or (un)substituted Ph; R20 represents hydrogen, or (un)substituted linear or branched C1-3 alkyl or R9 and R20 together forms C3-7 cycloalkyl; R10 represents hydrogen, (un)substituted linear or branched C1-3 alkyl; R11 represents hydrogen or (un)substituted linear or branched C1-3 alkyl, (un)substituted carbamoyl, or carboxy; R12 represents hydroxy or linear or branched C1-4 alkoxy; R13 represents hydrogen, (un)substituted linear or branched C1-6 alkyl, C2-6 alkenyl, or alkynyl, etc.; X, Y represents carbonyl or CH<sub>2</sub>; provisos are given.], which exhibit motilin receptor antagonism and being useful as drugs for preventing digestive tract movement or high level of blood motilin. Thus, 3-methyl-2-methylaminobutyric acid 2-(3-tert-butyl-4-hydroxyphenyl)-1-(2-pyridylcarbamoyl)ethylamide (prepn. given) was condensed with Boc-Phe(4-F)-OH using CMPI in the presence of Et<sub>3</sub>N in THF under ice-cooling for 4 h followed by treatment of the product with CF<sub>3</sub>CO<sub>2</sub>H in CH<sub>2</sub>Cl<sub>2</sub> gave 2-((2-amino-3-(4-fluorophenyl)propanoyl)-N-methylamino)-3-methylbutyric acid 2-(3-tert-butyl-4-hydroxyphenyl)-1-(2-pyridylcarbamoyl)ethylamide (II). II and N-Et-Phe(4-F)-N-Me-Val-N-Et-Tyr(3-tBu)-NH<sub>2</sub> showed IC<sub>50</sub> of 0.35 and 0.17 nM, resp., for inhibiting binding of <sup>125</sup>I-motilin to motilin receptor prepn. from mucus membrane of rabbit duodenum.

IT 287205-81-6P

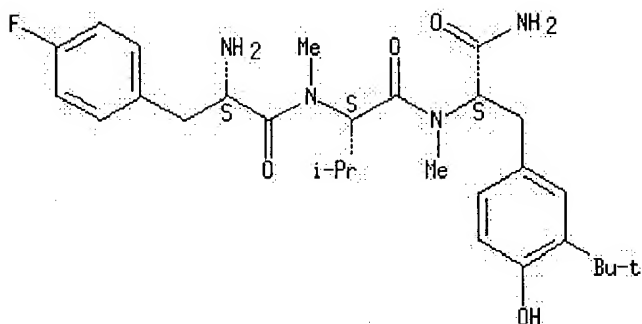
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of peptides or analogs contg. substituted phenethylamine moiety as motilin receptor antagonists and drugs for preventing digestive tract movement or high level of blood motilin)

RN 287205-81-6 HCAPLUS

CN L-Tyrosinamide, 4-fluoro-L-phenylalanyl-N-methyl-L-valyl-3-(1,1-dimethylethyl)-N $\alpha$ -methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

61.44

3369.55

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-1.40

-10.50

FILE 'CAOLD' ENTERED AT 23:44:54 ON 02 SEP 2004

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d his

(FILE 'HOME' ENTERED AT 21:22:36 ON 02 SEP 2004)

FILE 'REGISTRY' ENTERED AT 21:22:42 ON 02 SEP 2004

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 196 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 21:26:58 ON 02 SEP 2004

L4 STRUCTURE UPLOADED

S L4

FILE 'REGISTRY' ENTERED AT 21:28:05 ON 02 SEP 2004

L5 1 S L4



L6 FILE 'HCAPLUS' ENTERED AT 21:28:06 ON 02 SEP 2004  
 1 S L5

L7 FILE 'REGISTRY' ENTERED AT 21:28:09 ON 02 SEP 2004  
 STRUCTURE UPLOADED  
 L8 1 S L7

L9 FILE 'HCAPLUS' ENTERED AT 21:28:41 ON 02 SEP 2004  
 4 S L3

L10 FILE 'CAOLD' ENTERED AT 21:29:13 ON 02 SEP 2004  
 0 S L9

L11 FILE 'REGISTRY' ENTERED AT 21:29:19 ON 02 SEP 2004  
 STRUCTURE UPLOADED  
 L12 2 S L11  
 L13 352 S L11 FULL

L14 FILE 'HCAPLUS' ENTERED AT 21:31:02 ON 02 SEP 2004  
 7 S L13  
 L15 3 S L14 NOT L9  
 L16 1 S L15 AND MATSUOKA, H?/AU  
 L17 2 S L15 NOT L16  
 L18 1 S L17 AND SATO, T?/AU  
 L19 1 S L17 NOT L18  
 L20 0 S L19 AND TAKAHASHI, T?/AU  
 L21 0 S L17 AND KIM, D?/AU  
 L22 0 S L17 AND JUNG, K?/AU  
 L23 0 S L17 AND PARK, C?/AU  
 L24 0 S L19 AND KIM, D?/AU  
 L25 0 S L19 AND PARK, C?/AU

L26 FILE 'CAOLD' ENTERED AT 21:33:05 ON 02 SEP 2004  
 0 S L13

L27 FILE 'REGISTRY' ENTERED AT 21:33:13 ON 02 SEP 2004  
 STRUCTURE UPLOADED  
 L28 2 S L27  
 L29 STRUCTURE UPLOADED  
 L30 50 S L29  
 L31 15669 S L29 FULL

L32 FILE 'HCAPLUS' ENTERED AT 21:35:22 ON 02 SEP 2004  
 8855 S L31

L33 FILE 'REGISTRY' ENTERED AT 21:35:31 ON 02 SEP 2004  
 STRUCTURE UPLOADED  
 L34 50 S L33  
 L35 STRUCTURE UPLOADED  
 L36 0 S L35  
 L37 347 S L35 FULL

L38 FILE 'HCAPLUS' ENTERED AT 21:38:15 ON 02 SEP 2004  
 7 S L37  
 L39 0 S L38 NOT L14

L40 FILE 'REGISTRY' ENTERED AT 21:38:35 ON 02 SEP 2004  
 STRUCTURE UPLOADED  
 L41 2 S L40  
 L42 351 S L40 FULL

FILE 'HCAPLUS' ENTERED AT 21:41:36 ON 02 SEP 2004  
L43 7 S L42

FILE 'REGISTRY' ENTERED AT 21:41:41 ON 02 SEP 2004  
L44 STRUCTURE UPLOADED  
L45 50 S L44  
L46 STRUCTURE UPLOADED  
L47 2 S L46  
L48 351 S L46 FULL  
L49 STRUCTURE UPLOADED  
L50 2 S L49  
L51 380 S L49 FULL

FILE 'HCAPLUS' ENTERED AT 21:47:37 ON 02 SEP 2004  
L52 7 S L51

FILE 'REGISTRY' ENTERED AT 21:47:42 ON 02 SEP 2004  
L53 STRUCTURE UPLOADED  
L54 2 S L53  
L55 439 S L53 FULL

FILE 'HCAPLUS' ENTERED AT 21:50:36 ON 02 SEP 2004  
L56 10 S L55  
L57 3 S L56 NOT L43

FILE 'CAOLD' ENTERED AT 21:52:39 ON 02 SEP 2004  
L58 0 S L55

FILE 'REGISTRY' ENTERED AT 21:52:47 ON 02 SEP 2004  
L59 STRUCTURE UPLOADED  
L60 2 S L59  
L61 439 S L59 FULL

FILE 'HCAPLUS' ENTERED AT 21:57:31 ON 02 SEP 2004  
L62 10 S L61

FILE 'REGISTRY' ENTERED AT 21:57:38 ON 02 SEP 2004  
L63 STRUCTURE UPLOADED  
L64 2 S L63  
L65 STRUCTURE UPLOADED  
L66 STRUCTURE UPLOADED  
L67 2 S L66  
L68 STRUCTURE UPLOADED  
L69 1 S L68  
L70 STRUCTURE UPLOADED  
L71 0 S L70  
L72 STRUCTURE UPLOADED  
L73 0 S L72  
L74 10 S L72 FULL  
L75 STRUCTURE UPLOADED  
L76 0 S L75  
L77 0 S L74 NOT L61  
L78 STRUCTURE UPLOADED  
L79 0 S L78  
L80 0 S L78 FULL  
L81 STRUCTURE UPLOADED  
L82 0 S L81  
L83 0 S L81 FULL  
L84 STRUCTURE UPLOADED

L85 0 S L84  
 L86 0 S L84 FULL  
 L87 STRUCTURE UPLOADED  
 L88 0 S L87  
 L89 0 S L87 FULL  
 L90 STRUCTURE UPLOADED  
 L91 0 S L90  
 L92 STRUCTURE UPLOADED  
 L93 0 S L92  
 L94 0 S L92 FULL  
 L95 STRUCTURE UPLOADED  
 L96 0 S L95  
 L97 5 S L95 FULL

FILE 'HCAPLUS' ENTERED AT 22:40:59 ON 02 SEP 2004  
 L98 1 S L97

FILE 'CAOLD' ENTERED AT 22:41:17 ON 02 SEP 2004  
 L99 0 S L97

FILE 'REGISTRY' ENTERED AT 22:41:28 ON 02 SEP 2004  
 L100 STRUCTURE UPLOADED  
 L101 0 S L100  
 L102 0 S L100 FULL  
 L103 STRUCTURE UPLOADED  
 L104 1 S L103  
 L105 STRUCTURE UPLOADED  
 L106 0 S L105  
 L107 STRUCTURE UPLOADED  
 L108 0 S L107  
 L109 41 S L107 FULL

FILE 'HCAPLUS' ENTERED AT 22:56:53 ON 02 SEP 2004  
 L110 2 S L109

FILE 'CAOLD' ENTERED AT 23:00:44 ON 02 SEP 2004  
 L111 0 S L109

FILE 'HCAPLUS' ENTERED AT 23:00:59 ON 02 SEP 2004  
 L112 1 S 130:19658/DN  
 SEL RN

FILE 'HCAPLUS' ENTERED AT 23:01:37 ON 02 SEP 2004  
 L113 880326 S E1-E4

FILE 'REGISTRY' ENTERED AT 23:02:05 ON 02 SEP 2004  
 L114 4 S E1-E4

FILE 'REGISTRY' ENTERED AT 23:02:44 ON 02 SEP 2004

FILE 'HCAPLUS' ENTERED AT 23:03:10 ON 02 SEP 2004  
 L115 1 S 130:196958/DN  
 SEL RN

FILE 'REGISTRY' ENTERED AT 23:03:32 ON 02 SEP 2004

FILE 'HCAPLUS' ENTERED AT 23:03:38 ON 02 SEP 2004  
 DELETE SELECT  
 SEL RN

FILE 'REGISTRY' ENTERED AT 23:04:01 ON 02 SEP 2004

L116 276 S E1-E276  
 L117 STRUCTURE UPLOADED  
 L118 0 S L117  
 L119 0 S L118 FULL  
 L120 STRUCTURE UPLOADED  
 L121 2 S L120  
 L122 STRUCTURE UPLOADED  
 L123 2 S L122  
 L124 STRUCTURE UPLOADED  
 L125 1 S L124  
 L126 1 S L125  
 L127 353 S L125 FULL

FILE 'HCAPLUS' ENTERED AT 23:31:50 ON 02 SEP 2004

L128 4 S L127  
 L129 2 S L128 AND MATSUOKA, H?/AU

FILE 'CAOLD' ENTERED AT 23:44:54 ON 02 SEP 2004

=> s l127

L130 0 L127

=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.42	3369.97
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-10.50

FILE 'REGISTRY' ENTERED AT 23:45:20 ON 02 SEP 2004

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STRUCTURE FILE UPDATES: 1 SEP 2004 HIGHEST RN 737690-81-2  
 DICTIONARY FILE UPDATES: 1 SEP 2004 HIGHEST RN 737690-81-2

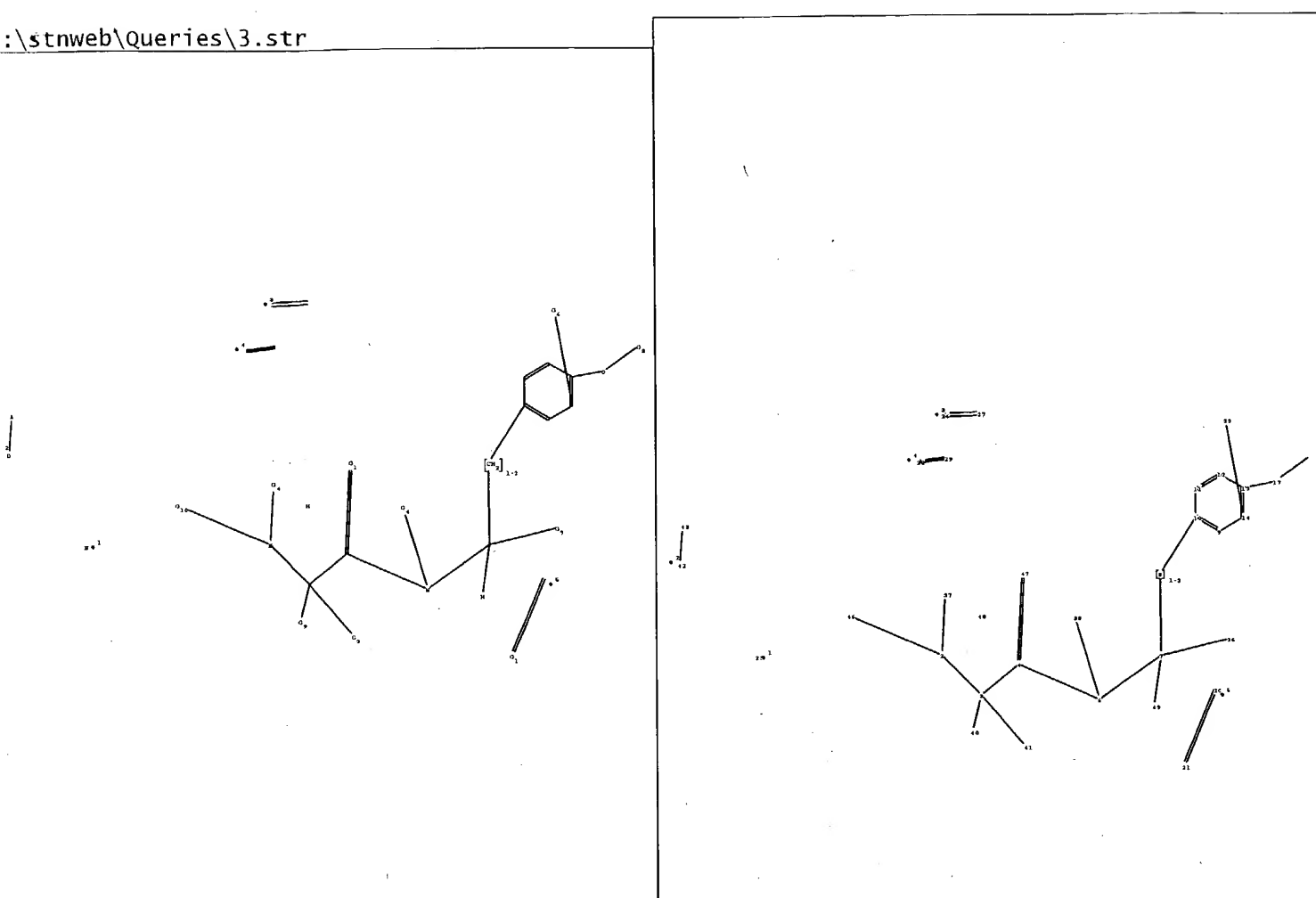
TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>



chain nodes :  
 2 3 4 6 7 8 17 20 21 23 26 27 28 29 33 36 37 38 40 41 42 43 46 47  
 48 49 50  
 ring nodes :  
 9 10 11 12 13 14  
 chain bonds :  
 2-37 2-3 2-46 3-4 3-40 3-41 4-6 4-47 6-7 6-38 7-8 7-36 7-49 8-10 13-17  
 14-33 17-50 20-21 26-27 28-29 42-43  
 ring bonds :  
 9-10 9-14 10-11 11-12 12-13 13-14  
 exact/norm bonds :  
 2-37 2-3 2-46 3-40 3-41 4-6 4-47 6-7 6-38 7-36 13-17 14-33 17-50 20-21  
 42-43  
 exact bonds :  
 3-4 7-8 7-49 8-10 26-27 28-29  
 normalized bonds :  
 9-10 9-14 10-11 11-12 12-13 13-14

G1:O,S

G2:CH3,Et

G3:H,Ak

G4:CH3,Et,H

G5:Ak,H,OH,[\*1],[\*2]

G6:Ak,Cb,[\*3],[\*4]

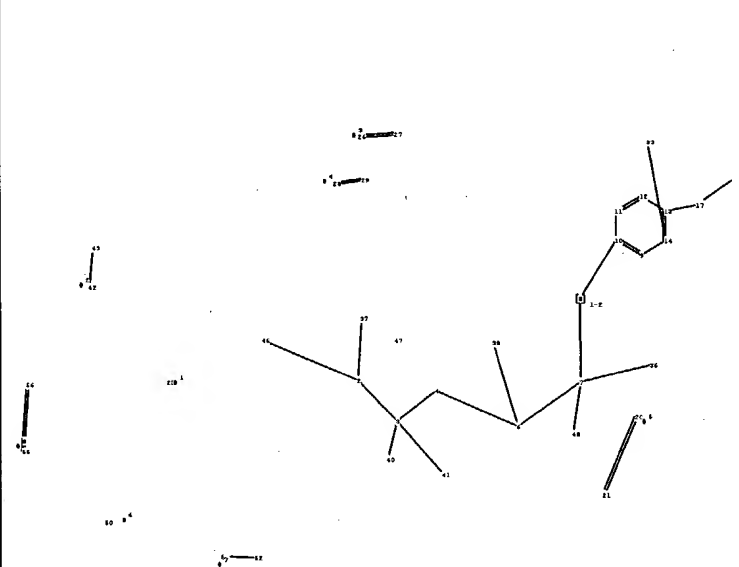
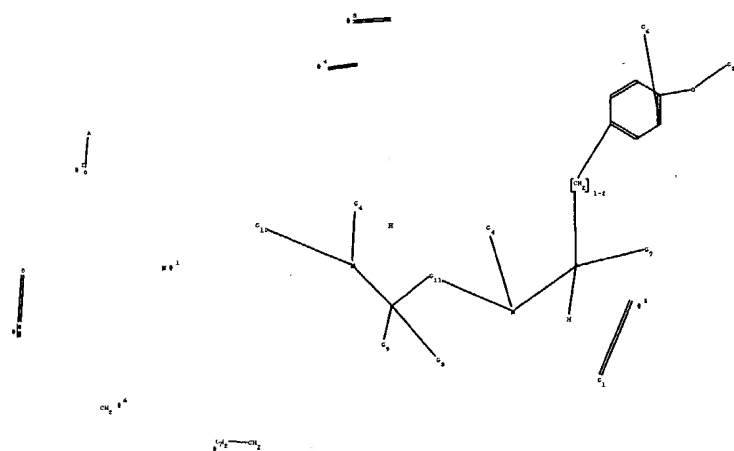
G7:COOH,Ak,H,[\*5]

G9:Ak,Ph

10:H,A

atch level :

2:CLASS 3:CLASS 4:CLASS 6:CLASS 7:CLASS 8:CLASS 9:Atom 10:Atom 11:Atom 12:Atom  
13:Atom 14:Atom 17:CLASS 20:CLASS 21:CLASS 23:CLASS 26:CLASS 27:CLASS 28:CLASS  
29:CLASS 33:CLASS 36:CLASS 37:CLASS 38:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS  
46:CLASS 47:CLASS 48:CLASS 49:CLASS 50:CLASS



chain nodes :

2 3 4 6 7 8 17 20 21 23 26 27 28 29 33 36 37 38 40 41 42 43 46 47  
48 49 50 51 52 55 56

ring nodes :

9 10 11 12 13 14

chain bonds :

2-37 2-3 2-46 3-4 3-40 3-41 4-6 6-7 6-38 7-8 7-36 7-48 8-10 13-17 14-33  
17-49 20-21 26-27 28-29 42-43 51-52 55-56

ring bonds :

9-10 9-14 10-11 11-12 12-13 13-14

exact/norm bonds :

2-37 2-3 2-46 3-40 3-41 4-6 6-7 6-38 7-36 13-17 14-33 17-49 20-21 42-43  
55-56

exact bonds :

3-4 7-8 7-48 8-10 26-27 28-29 51-52

normalized bonds :

9-10 9-14 10-11 11-12 12-13 13-14

G1:O,S

G2:CH3,Et

G3:H,Ak

G4:CH3,Et,H

G5:Ak,H,OH, [\*1], [\*2]

G6:Ak,Cb, [\*3], [\*4]

G7:COOH,Ak,H, [\*5]

G9:Ak,Ph

0:H,A

1:[\*6],[\*7],[\*8]

tch level :

2:CLASS 3:CLASS 4:CLASS 6:CLASS 7:CLASS 8:CLASS 9:Atom 10:Atom 11:Atom 12:Atom  
13:Atom 14:Atom 17:CLASS 20:CLASS 21:CLASS 23:CLASS 26:CLASS 27:CLASS 28:CLASS  
29:CLASS 33:CLASS 36:CLASS 37:CLASS 38:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS  
46:CLASS 47:CLASS 48:CLASS 49:CLASS 50:CLASS 51:CLASS 52:CLASS 55:CLASS 56:CLASS



\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 "Ask CAS" for self-help around the clock  
NEWS 3 May 12 EXTEND option available in structure searching  
NEWS 4 May 12 Polymer links for the POLYLINK command completed in REGISTRY  
NEWS 5 May 27 New UPM (Update Code Maximum) field for more efficient patent SDIs in CAplus  
NEWS 6 May 27 CAplus super roles and document types searchable in REGISTRY  
NEWS 7 Jun 28 Additional enzyme-catalyzed reactions added to CASREACT  
NEWS 8 Jun 28 ANTE, AQUALINE, BIOENG, CIVILENG, ENVIROENG, MECHENG, and WATER from CSA now available on STN(R)  
NEWS 9 Jul 12 BEILSTEIN enhanced with new display and select options, resulting in a closer connection to BABS  
NEWS 10 Jul 30 BEILSTEIN on STN workshop to be held August 24 in conjunction with the 228th ACS National Meeting  
NEWS 11 AUG 02 IFIPAT/IFIUDB/IFICDB reloaded with new search and display fields  
NEWS 12 AUG 02 CAplus and CA patent records enhanced with European and Japan Patent Office Classifications  
NEWS 13 AUG 02 STN User Update to be held August 22 in conjunction with the 228th ACS National Meeting  
NEWS 14 AUG 02 The Analysis Edition of STN Express with Discover! (Version 7.01 for Windows) now available  
NEWS 15 AUG 04 Pricing for the Save Answers for SciFinder Wizard within STN Express with Discover! will change September 1, 2004  
NEWS 16 AUG 27 BIOCOMMERCE: Changes and enhancements to content coverage  
NEWS 17 AUG 27 BIOTECHABS/BIOTECHDS: Two new display fields added for legal status data from INPADOC  
NEWS 18 SEP 01 INPADOC: New family current-awareness alert (SDI) available  
NEWS 19 SEP 01 New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!  
NEWS 20 SEP 01 New display format, HITSTR, available in WPIDS/WPINDEX/WPIX  
NEWS EXPRESS JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004  
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NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 14:13:41 ON 03 SEP 2004

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

h

eb c

g cg b

cg

eb

	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 14:13:47 ON 03 SEP 2004  
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STRUCTURE FILE UPDATES: 2 SEP 2004 HIGHEST RN 737922-52-0  
 DICTIONARY FILE UPDATES: 2 SEP 2004 HIGHEST RN 737922-52-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when  
 conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
 information enter HELP PROP at an arrow prompt in the file or refer  
 to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

=> s l1

SAMPLE SEARCH INITIATED 14:17:33 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 33736 TO ITERATE

3.0% PROCESSED	1000 ITERATIONS	2 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)		
SEARCH TIME: 00.00.01		

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
 BATCH \*\*INCOMPLETE\*\*

PROJECTED ITERATIONS: 663752 TO 685688  
 PROJECTED ANSWERS: 857 TO 1841

L2 2 SEA SSS SAM L1

=>

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*  
 SESSION RESUMED IN FILE 'REGISTRY' AT 14:24:21 ON 03 SEP 2004  
 FILE 'REGISTRY' ENTERED AT 14:24:21 ON 03 SEP 2004  
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	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	7.14	7.35

=>

L3 STRUCTURE UPLOADED

=> d 13  
 L3 HAS NO ANSWERS  
 L3 STR

=> s 13  
 SAMPLE SEARCH INITIATED 14:26:28 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 29316 TO ITERATE

3.4% PROCESSED 1000 ITERATIONS 1 ANSWERS  
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
 SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 576090 TO 596550  
 PROJECTED ANSWERS: 262 TO 910

L4 1 SEA SSS SAM L3

=>  
 L5 STRUCTURE UPLOADED

=> d 15  
 L5 HAS NO ANSWERS  
 L5 STR

=> s 15  
 SAMPLE SEARCH INITIATED 14:27:45 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 29316 TO ITERATE

3.4% PROCESSED 1000 ITERATIONS 0 ANSWERS  
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 576090 TO 596550  
 PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

=>  
 L7 STRUCTURE UPLOADED

=> s 17  
 SAMPLE SEARCH INITIATED 14:29:33 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 14078 TO ITERATE

7.1% PROCESSED 1000 ITERATIONS 0 ANSWERS  
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 274455 TO 288665  
 PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

=> s 17 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS  
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
 FULL SEARCH INITIATED 14:29:38 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 282169 TO ITERATE

100.0% PROCESSED 282169 ITERATIONS 0 ANSWERS  
 SEARCH TIME: 00.00.13

L9 0 SEA SSS FUL L7

=>  
 L10 STRUCTURE UPLOADED

=> d l10  
 L10 HAS NO ANSWERS  
 L10 STR

=> s l10  
 SAMPLE SEARCH INITIATED 14:32:06 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 15187 TO ITERATE

6.6% PROCESSED 1000 ITERATIONS 0 ANSWERS  
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 296362 TO 311118  
 PROJECTED ANSWERS: 0 TO 0

L11 0 SEA SSS SAM L10

=> s l10 full  
 THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS  
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
 FULL SEARCH INITIATED 14:32:11 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 303479 TO ITERATE

100.0% PROCESSED 303479 ITERATIONS 0 ANSWERS  
 SEARCH TIME: 00.00.14

L12 0 SEA SSS FUL L10

=> log y		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	323.02	323.23

STN INTERNATIONAL LOGOFF AT 14:32:36 ON 03 SEP 2004